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VOLUME VII

PRODUCTION OF JET FUELS FROM COAL DERIVED LIQUIDS

VOLUME VII -- GPGP JET FUELS PRODUCTION PROGRAM -- EVALUATION OF TECHNICAL UNCERTAINTIES FOR PRODUCING JET FUELS FROM LIQUID BY-PRODUCTS OF THE GREAT PLAINS GASIFICATION PLANT

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In September 1986, the Fuels Branch of the Aero Propulsion Laboratory at Wright-Patterson Air Force Base, Ohio, commenced an investigation of the potential of jet fuel production from the liquid by-product streams produced by the gasification of lignite at the Great Plains Gasification Plant (GPGP) in Beulah, North Dakota. Funding has been provided by the Department of Energy (DOE) Pittsburgh Energy Technology Center (PETC) to administer the experimental portion of this effort. This document reports the results of the effort by Burns and Roe Services Corporation/Science Applications International Corporation (BRSC/SAIC) to analyze GPGP operations and develop correlations for the liquid by-products and plant operating factors such as coal feed rate and coal characteristics. This report discusses those parameters which are predictors of by-product production as well as the variability of the by-product production.

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FOREWORD

In September 1986, the Fuels Branch of the Aero Propulsion Laboratory at Wright-Patterson Air Force Base, Ohio commenced an investigation of the potential of production of jet fuel from the liquid by-product streams produced by the gasification of lignite at the Great Plains Gasification Plant (GPGP) in Beulah, North Dakota. Funding was provided to the Department of Energy (DOE) Pittsburgh Energy Technology Center (PETC) to administer the experimental portion of this effort. This report details the effort of Burns and Roe Services Corporation/Science Applications International Corporation (BRSC/SAIC), who, as a contractor of DOE (DOE Contract No DE-AC22-84PC72571), analyzed plant operating data and developed correlations of the liquid by-product yields from the GPGP. DOE/PETC was funded through Military Interdepartmental Purchase Request (MIPR) FY1455-86-N0657. Mr. William E. Harrison III was the Air Force Program Manager and Mr. Gary Stiegel was the DOE/PETC Program Manager.

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1.0 EXECUTIVE SUMMARY

The Great Plains Gasification Plant (GPGP) represents the first commercial Synfuels Plant in the United States. The plant is currently being operated for the Department of Energy (DOE) by the ANG Coal Gasification Company to produce synthetic natural gas (SNG) from North Dakota lignite. Although the plant was designed to nominally produce 137.5 MMSCF of SNG per day, ANG has more recently operated at an average rate approaching 150 MMSCF SNG per day. In addition to SNG, the GPGP also produces three liquid hydrocarbon by-product streams: Rectisol naphtha, crude phenol, and tar oil. While these by-product liquids have a potential market value as transportation fuels and/or chemicals, they are currently burned in the plants boilers as fuels.

In 1986, the Department of Defense and DOE kicked-off a program aimed at assessing the feasibility of producing specification jet fuels from the GPGP by-products, and in particular, the tar oil. Because it is known that the naphtha and crude phenol streams contain potentially valuable chemicals, the Jet Fuels Production Program is also investigating the feasibility of recovering these chemicals as co-products and selling them to subsidize the production of jet fuels. It is important to assess the variability of the by-product yield during plant operations in order to be able to predict by-product yields as a function of future plant operating conditions and thus assist the design and economic assessment of the Jet Fuels Production Facility. ANG has consistently monitored by-product production rates as well as key operating parameters since 1985. The specific purpose of the work discussed in this report was to analyze plant operating data and develop correlations of the liquid by-product yields from the GPGP. Important variables controlling the production of these by-products were to be identified and the results utilized to estimate the technical uncertainties associated with the production of such feedstocks.

This study concludes that the production of SNG, naphtha, crude phenol, and tar oil is most strongly influenced by the moisture and ash free

(MAF) coal feed rate. It was also determined that coal characteristics such as volatile matter, H/C ratio, sulfur, ash, and Na_2O content, and ash fusion temperature did not contribute to a better correlation for SNG production. With the exception of the atomic H/C ratio of the feed coal, this was also true for the tar oil, crude phenol, and naphtha.

In the case of the tar oil, yields decreased with increased coal H/C ratio, while phenol increased slightly with an increase in coal H/C ratio. This study also concludes that it is not currently possible to explain all the variation in production on the basis of available data. One particular limitation regards the restricted nature of key gasifier operating parameters such as oxygen-to-steam ratios, temperatures, pressures, and solids residence time. While these data may have aided development of more comprehensive by-product correlations, they are proprietary and not generally available. Lastly, independent analysis and comparison of the 1987 by-product yields to the 1985-86 yields indicates that the 1987 data on production do not appear to be significantly different than the 1985-1986 data.

As a result of this effort to analyze liquid by-product production as a function of operating parameters, several recommendations have been proposed. These include further study and analysis of basic processes governing liquids production in the gasifier; analyses of downstream operations that possibly influence liquid yield and quality; and detailed investigation of the relationship between coal feed rate, gasifier operation, coal characteristics, by-product production and by-product characteristics. Finally, it is also suggested that the correlations developed in this study be utilized in the technical and economics feasibility studies developing an optimum design for the jet fuel production facilities.

2.0 GOALS AND OBJECTIVES

As part of the Jet Fuels Production Program, the Department of Defense (DOD), and Department of Energy (DOE) requested BRSC/SAIC to review and

analyze GPGP by-product production data and coal characterization data for the period from the second quarter of 1985 through January 1987. The objective of this work was to develop useful correlations that could be used to predict the quantities of by-products produced by the plant. Important variables that could perhaps be used to control the amounts of the by-products were to be identified. From the statistical analysis of the data, technical uncertainties associated with the production of the feedstocks for jet fuel manufacture could be identified, quantified, and considered in the design of the jet fuel facilities.

3.0 APPROACH

The scope of the work done in the data correlation area included the development of correlations for the tar oil production and the phenol production. Correlations were also developed for SNG production and naphtha since they might provide information regarding important controlling variables. Correlations for these variables were also needed to predict the possible effects of changing parameter values. The data base used comprised the data contained in the GPGP progress reports. These reports include data on product yields and feed coal characteristics, but do not include data on gasifier operating conditions, which are not generally available.

The correlation work was done in two phases: an initial preliminary phase to identify important variables and develop correlations, and a secondary phase to test the correlations with the latest, best data. Each phase is described in the report, including the development of the data base, identification of correlating variables, development of the correlations, and the results.

4.0 PRODUCTION OF LIQUIDS IN GASIFICATION SYSTEMS

Since the main objective of operating a coal gasifier is usually to produce gas, little attention has been paid to the production of liquid by-products in such systems. The usual objective in dealing with

liquid by-products is to minimize or eliminate them. In some gasifier designs essentially no liquids are produced, and even in the case of the Lurgi system, the literature suggests that tar and oil can be recycled to extinction in the gasifier. Thus, data on liquid by-product production in coal gasifiers have not been collected and analyzed in detail to determine the underlying variables and their effects on liquid production. In the case of the GPGP Lurgi gasifiers, the operating data are proprietary and are not currently available; only a few isolated example runs are reported in the literature to support a general description of the system.

However, the literature (1,2,3,4,5,6) does make the point that in a gasifier coal is heated through the temperature regime where pyrolytic reactions occur, and a knowledge of the kinetics of coal pyrolysis is essential in predicting the yield and products distribution in a coal gasifier. In the case of a moving bed gasifier such as the Lurgi, the reactor is viewed as comprising four reaction zones. These zones are illustrated in Figure 1, which also shows typical temperature ranges and associated reactions within the zones.

The reaction gases travel up through the bed countercurrent to the coal moving slowly downward. The gases are heated in the combustion zone and then enter the gasification zone. Gases leaving the gasification zone, where reduction reactions occur, are substantially cooler because of the endothermicity of these reactions. Gas entering the devolatilization zone then gives up sensible heat to heat the coal to pyrolysis temperatures and to produce the heat required for pyrolysis reactions. Cooled gas from this exchange, now carrying the products of pyrolysis, rises through the incoming fresh coal to preheat and dry it. To some extent, heavy pyrolysis products are believed to condense out in the drying zone to aid in heat transfer. The result is a recycle of heavier hydrocarbons to devolatilization, there to be revolatilized and partially pyrolyzed. Cooled product gases leave the bed at the dew point temperature (highly variable, but nominally about 900-1000°F).

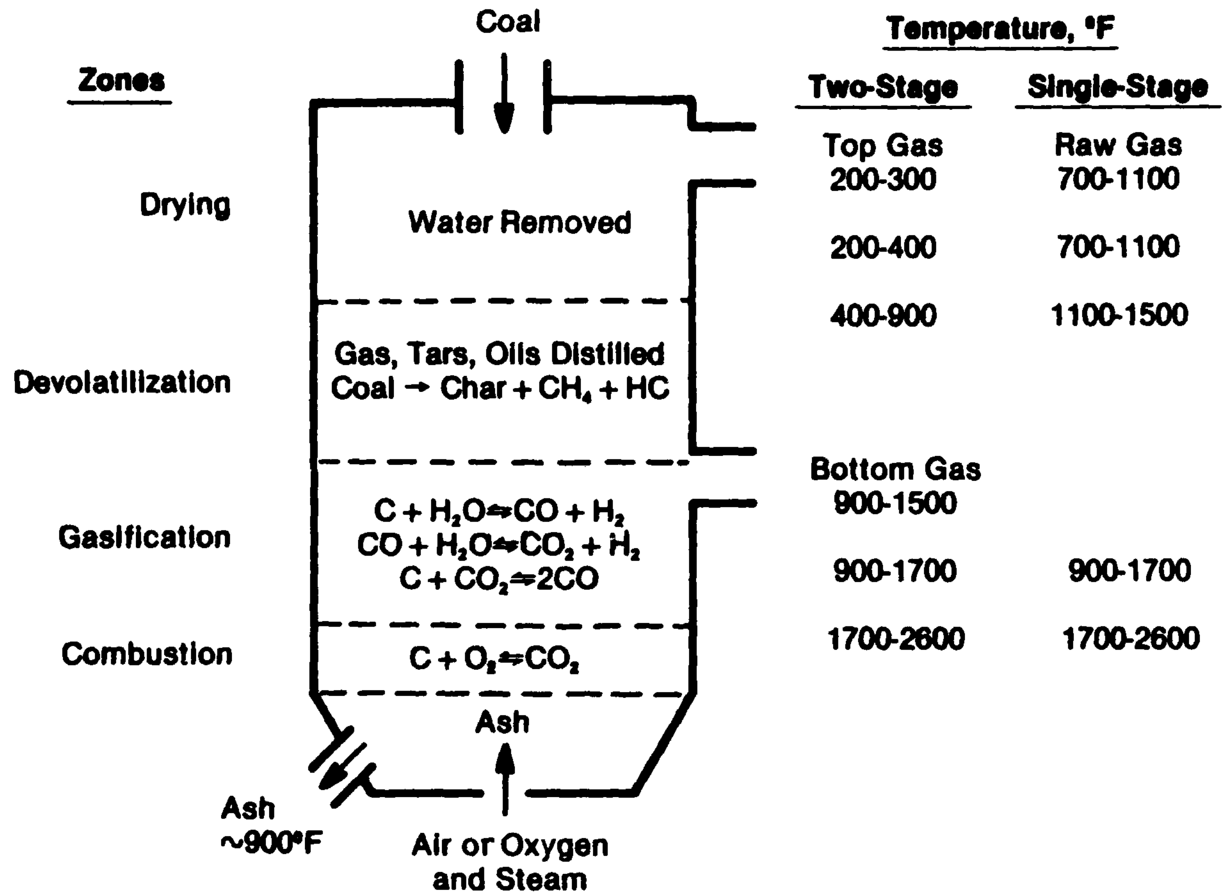

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FIGURE 1. CHEMICAL REACTIONS AND TEMPERATURES IN MOVING BED GASIFIER.

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Solid coal passes successively downward through the zones, being heated all the way, first for drying, next devolatilization followed by char reduction, and then oxidation; finally, the residues are cooled by incoming steam-oxygen before the ash is discharged via the grate. In the devolatilization zone gaseous products are formed as weak bonds in the coal structure are ruptured, and these gaseous products are removed from the gasifier with the gases from the combustion and gasification zones. The temperature of the exiting mixture is not high enough for the rapid thermal decomposition of the volatile matter. The volatile matter by-products can be divided into water-soluble compounds, such as phenols, ammonia, and fatty acids, and water-insoluble components, such as tars, oils, and naphtha.

From this model of the reactor and the reaction zones, it appears that the tar and tar oil are formed in the devolatilization zone as the result of primary pyrolytic reactions and secondary cracking or polymerization reactions of the primary volatiles. Information on correlation of yields with feed material properties and important operating variables can then perhaps be found from the extensive literature on coal pyrolysis. Some of this literature was searched, and some important variables were identified. Where data were available on these variables, correlations were attempted, as discussed in the next sections. Identification of parameters that may be important in controlling the production of tar, tar oil, and phenol in the Lurgi system would also be useful for identifying types of data that may be useful to collect from the GPGP. However, the main objective at GPGP is to produce gas so that there may be relatively slight opportunity to manipulate certain operating parameters to determine their effect on liquid by-product production.

Important parameters found to influence the yield and distribution of liquid products from gasification/pyrolysis reactions include the following:

o Temperature

- Rate of heating (slow vs. fast)
- Pressure
- Volatile matter content of feed coal
- Hydrogen/carbon ratio of feed coal
- Particle size of feed coal

Data are not available from the GPGP on the primary process-control variables of oxygen rate and the steam-to-oxygen ratio, which would control the temperature and rate of heating. Data on pressure are similarly not available. Two of the other parameters shown were used as correlating variables. Data should perhaps be obtained in the future on the particle size of the feed coal on a regular basis.

Because the available data on liquid by-product production are for the plant output rather than the reactor output, a number of other operating variables should be examined, such as the proportion of the gas going through the shift converter. Hydrogenation within this unit affects the quality and quantity of the by-products.

5.0 INITIAL CORRELATION WORK

The initial preliminary work which was done to develop data correlations was based on data from GPGP from 1985 and 1986, and was aimed at identifying important variables. The following discussion summarizes the results of this phase of the work.

5.1 Data Base Development

The basic GPGP data base that was available for the initial work phase consisted of the daily data contained in the quarterly progress reports from the Second Quarter 1985 through the Third Quarter 1986, and additional daily data by month contained on three PC diskettes from January 1986 through January 1987. Depending on the variables of interest, not all types of data were available on a daily basis. For example, feed coal composition

data, including volatile matter and ultimate analysis, were available for only one out of every three or four days. In addition, a few data points were either missing or obviously in error. Thus, depending on the types of correlations to be developed and compared, the data base was examined and appropriate data sets were selected. The data were inserted into a spreadsheet format (Lotus 1-2-3™, Release 1a) on a PC for analysis, manipulation, and presentation.

The data that were available on a daily basis, and entered into a data base, termed the large data base, included:

- Date
- Coal delivered
- Percent moisture, a.r. (as received)
- Percent ash, dry
- Percent sulfur, dry
- SNG production (MIS,Net)
- Tar oil production
- Naphtha production
- Phenol production

This data base included approximately 530 data sets.

Data on feed coal composition were not available on a daily basis as they were obtained only once every three or four days. In addition, not all data of this type were available on the same day. For the purposes of comparing correlations based on different variables, it was desired to obtain a coherent data base with all the variables in each data set that might be of interest. Consequently, the data sets were screened to make sure that all variables were represented in each data set. A data base was thus developed, termed the small data base, which included the following variables in addition to those listed above:

- Percent volatile matter
- Percent carbon, maf (moisture, ash-free)
- Percent hydrogen, maf (moisture, ash-free)
- Average number of gasifiers operating

This data base included approximately 150 data sets. In addition to using primary data variables directly as correlating variables, correlating variables such as atomic H/C ratio, maf coal feed rate, and liquid produced/ton coal were derived from the primary data variables.

5.2 Preliminary Identification of Correlating Variables

The initial effort in the preliminary phase was aimed at correlating the tar oil production with a number of the primary data variables contained in the large data base. Because basic data on gasifier operating conditions were not available, the SNG production rate was chosen, also, as correlating variable for tar oil production; it was thought that SNG production might be a variable representative of gasification reaction severity. Correlations were developed, using standard statistical methods (7), for tar oil production as the dependent variable and the following sets of independent variables:

- SNG production
- Maf coal feed rate
- Maf coal feed rate and SNG production
- Maf coal feed rate and percent sulfur
- Maf coal feed rate and percent ash

The results are summarized in Table A-1 in the appendix. Table A-2 lists some characteristics of the data.

The most significant correlation of the tar oil production with one variable was with the maf coal feed rate, rather than SNG

production, as shown by a slightly higher sum of squares removed by the correlation. Including both of these variables as independent variables improved the correlation slightly, although SNG production is obviously highly correlated with maf coal feed rate. Including highly correlated independent variables in a correlation usually does not improve the correlation significantly.

A very small improvement in the correlation was obtained by including either the percent sulfur (maf) or the percent ash (maf) of the feed coal along with the maf coal feed rate as independent variables. This small improvement was not significantly, however, so that for all practical purposes, the best correlation of the tar oil production from the list above was with the maf coal feed rate as the one independent variable.

To try to produce a better correlation of tar oil production and maf coal feed rate, three-day rolling averages for both quantities were used to smooth out daily variations caused by the way tar oil production is measured. The initial data were smoothed considerably, as shown by the initial sum of the squares of deviations. The resulting least-squares regression was considerably better in terms of the fraction of the sum of the squares of deviations removed by correlation, and the confidence limits of the regression would be smaller. However, the correlation itself was not greatly different from the one developed by working with the original daily data. It was concluded that it was not necessary or useful to first smooth the daily data by calculating rolling averages.

To proceed further with the identification of important correlating variables, a number of different correlations with one independent variable were calculated from the small data base, which included data on feed coal characteristics. The dependent variables included SNG production, tar oil production, naphtha production, and phenol production. The independent variables

included maf coal feed rate, percent volatile matter in the feed coal, atomic H/C ratio of the feed coal, volatile matter feed rate, and number of gasifiers operating. This latter variable was looked at because it is proportional to reactor volume and thus can perhaps represent the effects of residence time on the progress of the reactions and product yields.

The objective of this analysis was to identify and rank correlating variables for each dependent variable in terms of the sum of squares of deviations removed by the correlation. The important variables found from this analysis could then be combined to develop the best overall correlation for each dependent variable. The numerical results are shown in Table A-3 in the appendix. The important conclusions are discussed below.

1. The maf coal feed rate was the most important correlating variable for each of the four dependent variables.

2. The volatile matter feed rate was in some cases equal in important to the maf coal feed rate, but as these two variables are highly correlated themselves, it would not be useful to include both of them as correlating variables.

3. Percent volatile matter did not help in correlating any of the dependent variables.

4. Atomic H/C ratio appeared to be a useful correlating variable for tar oil production and phenol production.

5. Number of gasifiers operating was a significant correlating variable for SNG production and tar oil production. However, this variable is highly correlated with coal feed rate.

These results composed the basis for selecting which correlations should be developed. The correlations that were developed in this initial phase are discussed in the sections below.

5.3 Correlations with One Independent Variable

Based on the effect discussed above to evaluate the relative significance of the possible independent correlating variables, it was concluded that the most important variable by far was the coal (maf) feed rate. Consequently, correlations were developed for the four plant products with this single correlating variable. These correlations were developed from the large data base described above containing 529 points. For SNG production and naphtha production, these correlations are the only useful ones which could be developed from the .,ailable data. For production of tar oil and phenol, these one-variable correlations may be useful in the absence of data on the feed coal characteristics, although including these latter data in the correlation results in a more accurate estimation, as discussed below.

Table A-5 in the Appendix lists the important parameters of these four correlations of the plant products with the maf coal feed rate with the characteristics of the data used for the correlations shown in Table A-6. The data are plotted along with the correlations in Figures A-1 (SNG production), A-2 (tar oil production), A-3 (naphtha production), and A-4 (phenol production).

5.4 Correlations with Two Independent Variables

As explained in Section 5.2, it was found that correlations for tar oil production and phenol production could be improved by including the feed coal atomic H/C ratio as an additional correlating variable along with coal (maf) feed rate. Consequently, correlations were developed from the smaller data base for tar oil production and phenol production with these two variables as the

independent correlating variables. In addition, to illustrate the dependence of the production of tar oil and phenol on atomic H/C ratio, correlations were developed for the tar oil production and phenol production per ton of coal (maf) as a function of atomic H/C ratio. Although these latter correlations may be linear in only one independent variable, the atomic H/C ratio, the correlations are actually a function of two independent variables, the dependence with respect to the maf coal feed rate having been fixed by dividing it into the by-product production rate.

Table A-7 lists the important parameters of these correlations with the characteristics of the data used for the correlation shown in Table A-8. The correlation of tar oil production with coal (maf) feed rate and atomic H/C ratio is plotted in Figure A-5 along with the data points for the smaller data base. Another way of looking at the dependence of tar oil production upon the atomic H/C ratio of the feed coal is to plot the tar oil production per ton of coal (maf) versus the H/C ratio. This plot is shown in Figure A-6, which shows that the tar oil produced per ton of feed coal (maf) decreases as the atomic H/C ratio of the feed coal increases. Two correlations were calculated for these data: one which is linear in atomic H/C ratio and another which includes a second-order term, $(H/C)^2$. The second-order correlation was somewhat better. Both correlations are shown in Figure A-6.

The correlation of phenol production with coal (maf) feed rate and atomic H/C ratio is plotted in Figure A-7, along with the data points for the smaller data base. In a manner similar to the analysis of the tar oil production, the phenol production per ton of coal (maf) was plotted against the atomic H/C ratio. This plot is shown in Figure A-8, which shows that the phenol produced per ton of feed coal (maf) increases somewhat as the atomic H/C ratio of the feed coal increases. A linear least-squares correlation was calculated for this relationship and is plotted in Figure A-8.

6.0 FINAL CORRELATIONS

The second phase of the correlation work involved analyzing GPGP data from the first four months of 1987, and comparing them with the 1985-1986 data and the results of the first correlation effort. The following discussion summarizes the results of this second phase and the final correlations developed from the combined data.

6.1 Data Base Development

GPGP data from the first four months of 1987 were supplied to ANG in the form of files of data by month in spreadsheet format on several PC diskettes. The diskettes were first read to determine their contents in terms of variables. The monthly files were then combined to develop a comprehensive data base of 1987 data with consistent variables.

For a combined comparison and analysis the 1987 data were added to the 1985-1986 data. Two such combined data bases were developed. The so-called large data base, which contained a total of 645 data sets, was built upon the large 1985-1986 data base described above in Section 5.1. The primary purpose of this data base was to develop the product correlations with the maf coal feed rate.

A small 1987 data base was also developed containing the data on feed coal composition. Again, these types of data were not available on a daily basis, being obtained only once every three or four days. This data base was used to investigate the potential inclusion of a number of variables besides feed coal composition, such as ash fusion temperature, and a so-called small data base was put together which combined the 1987 and the 1985-1986 data. This combined small data base contained 163 or 190 data sets depending on which variables were being examined.

6.2 Identification of Correlating Variables

The identification of correlating variables in the combined data bases was, of course, guided by the results from the first phase. The small and the large combined data bases were used to generate graphs of each product's production versus potential correlating variables. The graphs were generated with different symbols for the two types of data -- 1985-1986 and 1987 -- in order to compare the two sets of data.

One objective of examining these graphs was to determine if the newer data really were different from the earlier data. In general, the 1987 data did not appear to be significantly different from the 1985-1986 data, and as a result final correlations were developed from the total combined data base instead of only the 1987 data. In addition, the 1987 data generally covered a smaller range of variation in the independent variable, making it more difficult to develop correlations with reasonable confidence limits on the basis of the newer data alone.

In an effort to find additional correlating variables besides maf coal feed rate and H/C atomic ratio, graphs were generated with an ash fusion temperature (IT or FT), weight percent Na_2O in coal (mf), or lignite carbon number as the independent variable. The ash fusion temperature was tried as a variable because it is though that variations in this variable would cause and therefore reflect a variation in gasifier steam rate. Weight percent Na_2O was tried because it was thought that this ash component might have a catalytic effect upon the gasification reactions.

Graphs were generated from the data bases for a number of dependent variables using ash fusion temperature as the independent variables: SNG production, SNG per ton of feed coal, tar oil production, tar oil per ton, phenol per ton, and naphtha

per ton. None of these graphs showed that any of these quantities had any correlation with ash fusion temperature.

Similarly, graphs with weight percent Na_2O or the lignite carbon number as the independent variable showed no correlation.

On the other hand, graphs generated with the independent variables found from the first phase to be useful correlating variables looked very much the same as the graphs with the 1985-1986 data. These independent correlating variables included maf coal feed rate and atomic H/C ratio.

6.3 Correlations with One Independent Variable

Based on the effort described in Section 5.2 and above to identify correlating variables, the most important variable is the maf coal feed rate. Correlations were developed for each of the four main plant products with this correlating variable. For SNG production and naphtha production, these correlations were the only ones which could be developed from the available data. Table 1 lists the important parameters of these four correlations of the plant products with the maf coal feed rate with the characteristics of the data used for the correlations shown in Table 2. The correlations in Table 1, which include the 1987 data, can be compared with the correlations in Table A-5 developed from the earlier data.

6.3.1 SNG Production. The two sets of SNG data are plotted in Figure 2, and it can be seen that the two sets overlap. Although the two sets of data overlap as if there were no significant difference between them, the data in the two sets are different types of numbers. The 1985-1986 data are MIS Net figures taken from the published progress reports whereas the 1987 data in the data base are the sum

Table 1. Parameters of Final Correlations of Plant Products vs. the Maf Coal Feed Rate

Dependent Variable	Independent Variable	Data Set	Intercept a	Slope b	Sum of Squares Removed	r^2
SNG production, MMSCFD	Maf coal feed rate, M tons/day	1987 116 pts.	5.31437	15.0912	18975.2	0.8078
Tar oil production, M gal/day	Maf coal feed rate, M tons/day	Combined 645 pts.	46.5664	8.89910	92659.9	0.2634
Naphtha production, M gal/day	Maf coal feed rate, M tons/day	Combined 645 pts.	2.26738	2.73966	8781.99	0.3599
Phenol production, M gal/day	Maf coal feed rate, M tons/day	Combined 645 pts.	10.0519	2.62406	8056.56	0.2801

Table 2. Characteristics of Data Used for Final Correlation (Table 2-1)

Variable	Average	Minimum	Maximum	Sum of Squares of Deviations $\Sigma(y-\bar{y})^2$ or $\Sigma(x-\bar{x})^2$
1987 Data Set (116 pts.):				
SNG, MMSCFD	146.869	33.5109	156.322	23489.2
Maf coal feed rate, Mtons/day	9.37996	3.44403	10.3749	83.3182
Combined Data Set (645 pts.):				
Tar Oil, Mgal/day	121.875	14.116	200.698	351850.
Naphtha, Mgal/day	25.4518	4.16	37.6	24402.8
Phenol, Mgal/day	32.2581	9.66	51.45	28762.0
Maf coal feed rate, Mtons/day	8.46252	3.4403	10.7572	1170.04

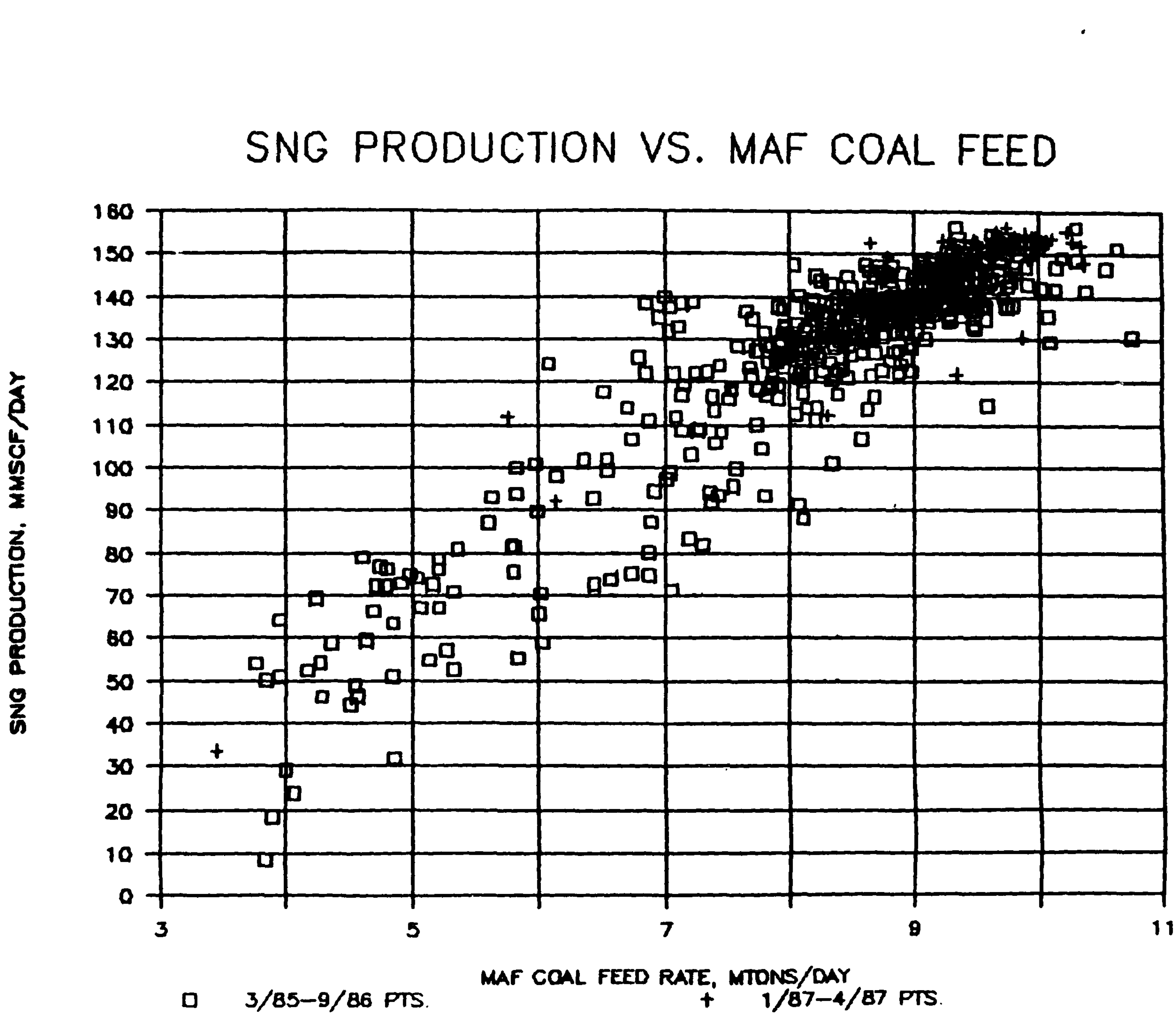

FIGURE 2. SNG Production vs. Maf Coal Feed Rate--Combined Large Data Base

of the quantity of SNG billed and that which was consumed internally. The latter figures are usually a few percent higher than the corresponding MIS Net numbers. Consequently, the 1987 SNG data, shown in Figure 3, were correlated by themselves, and the correlation line is also shown in Figure 3. The parameters of the calculated correlation line are shown in Table 1 and the detailed characteristics are shown in Table A-9 in the Appendix. The correlation coefficient r is 0.90, which is highly significant statistically (meaning that there is a correlation with little chance of being wrong) with 114 degrees of freedom.

6.3.2 Tar Oil Production. The two sets of tar oil production data are plotted in Figure 4, and it can be seen that the two sets overlap with no apparent significant difference between them. Consequently, all of the data in both sets were used to calculate a correlation of tar oil production as a function of maf coal feed rate. The parameters of the calculated correlation are shown in Table 1, and the detailed characteristics are shown in Table A-10 in the Appendix. The correlation coefficient r is 0.51, which is highly significant statistically with 643 degrees of freedom. The correlation explains only 26.3 percent of the sum of squares of deviations, however, meaning that other variables as yet unidentified (as well as a great deal of random variation caused by the way in which tar oil production is measured) play a role in determining tar oil production. The 1987 data are plotted in Figure 5, which also shows the correlation line.

6.3.3 Naphtha Production. The two sets of naphtha production data are plotted in Figure 6, and it can be seen that the two sets overlap with no apparent significant difference between them. Consequently, all of the data in both sets

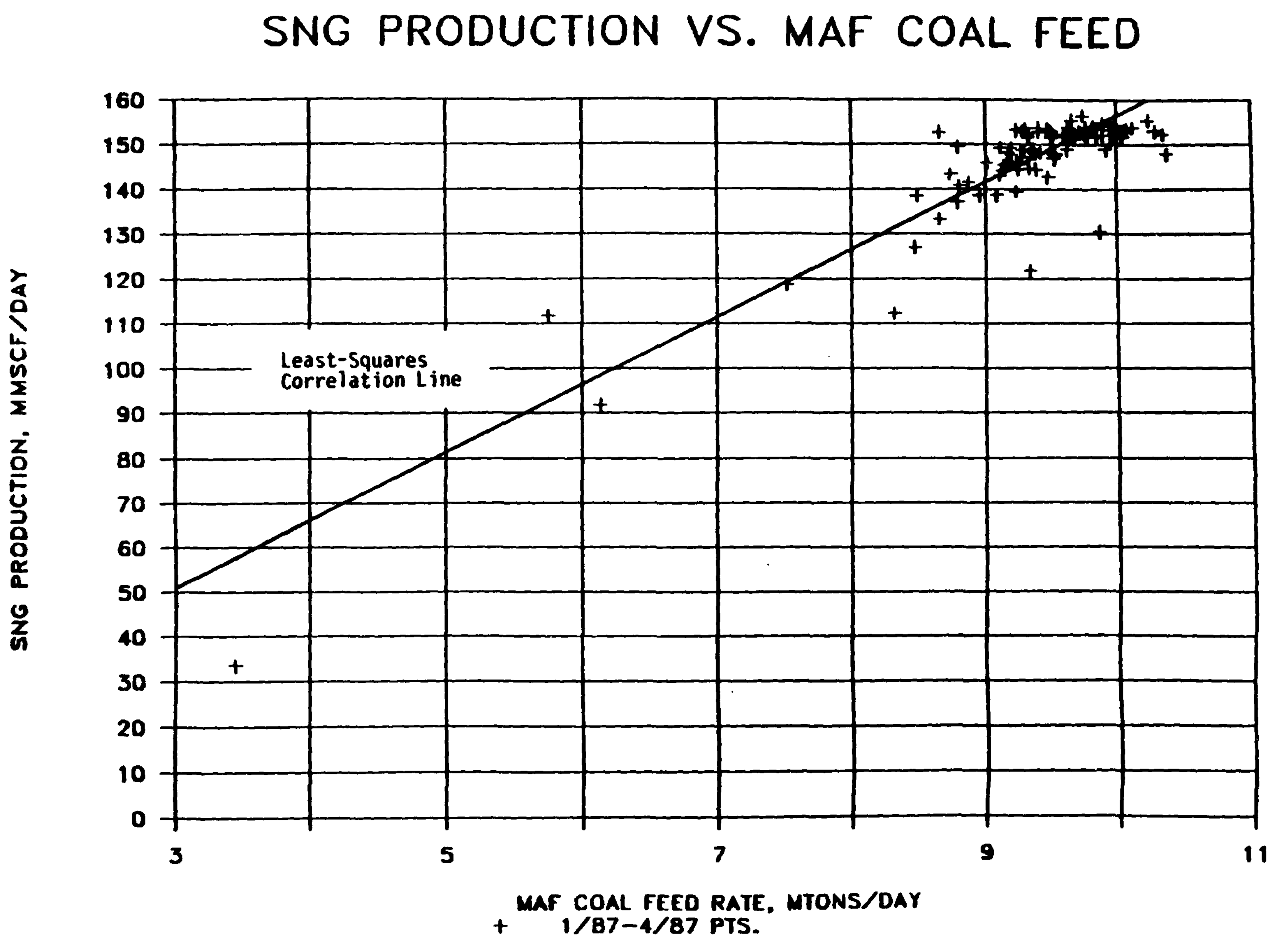

FIGURE 3. SNG Production vs. Maf Coal Feed Rate--1987 Data

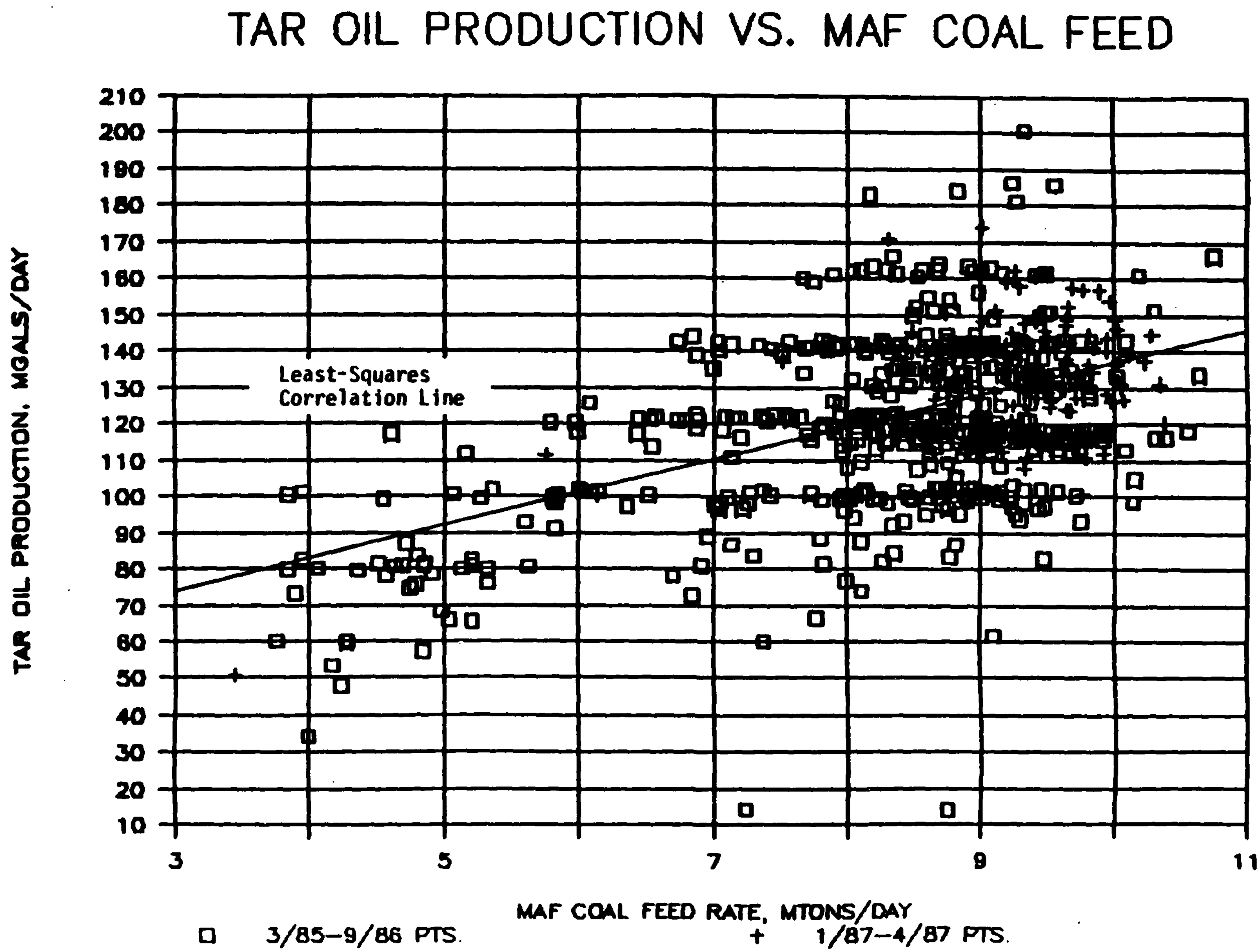

FIGURE 4. Tar Oil Production vs. Maf Coal Feed Rate--Combined Large Data Base

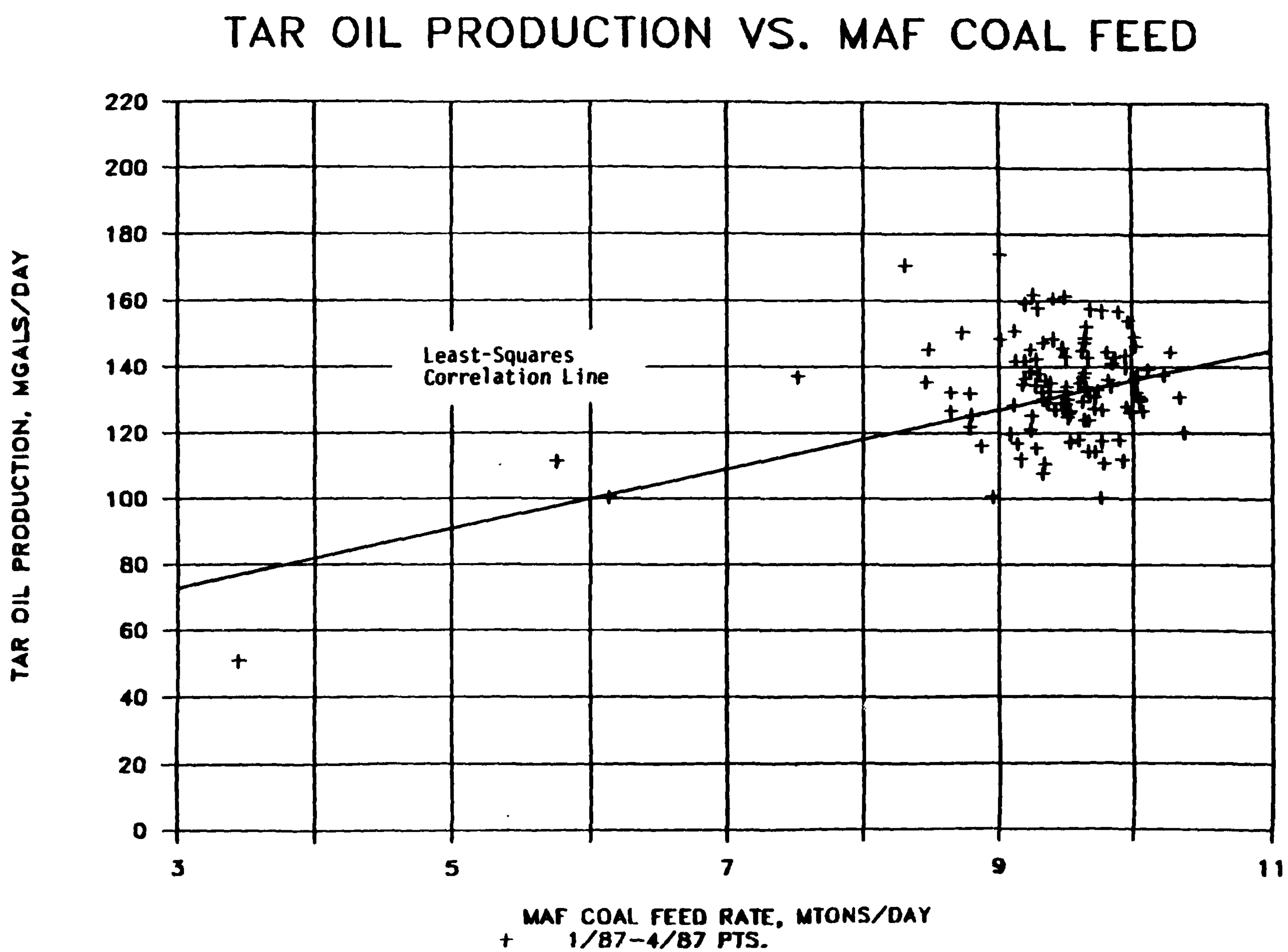

FIGURE 5. Tar Oil Production vs. Maf Coal Feed Rate--1987 Data

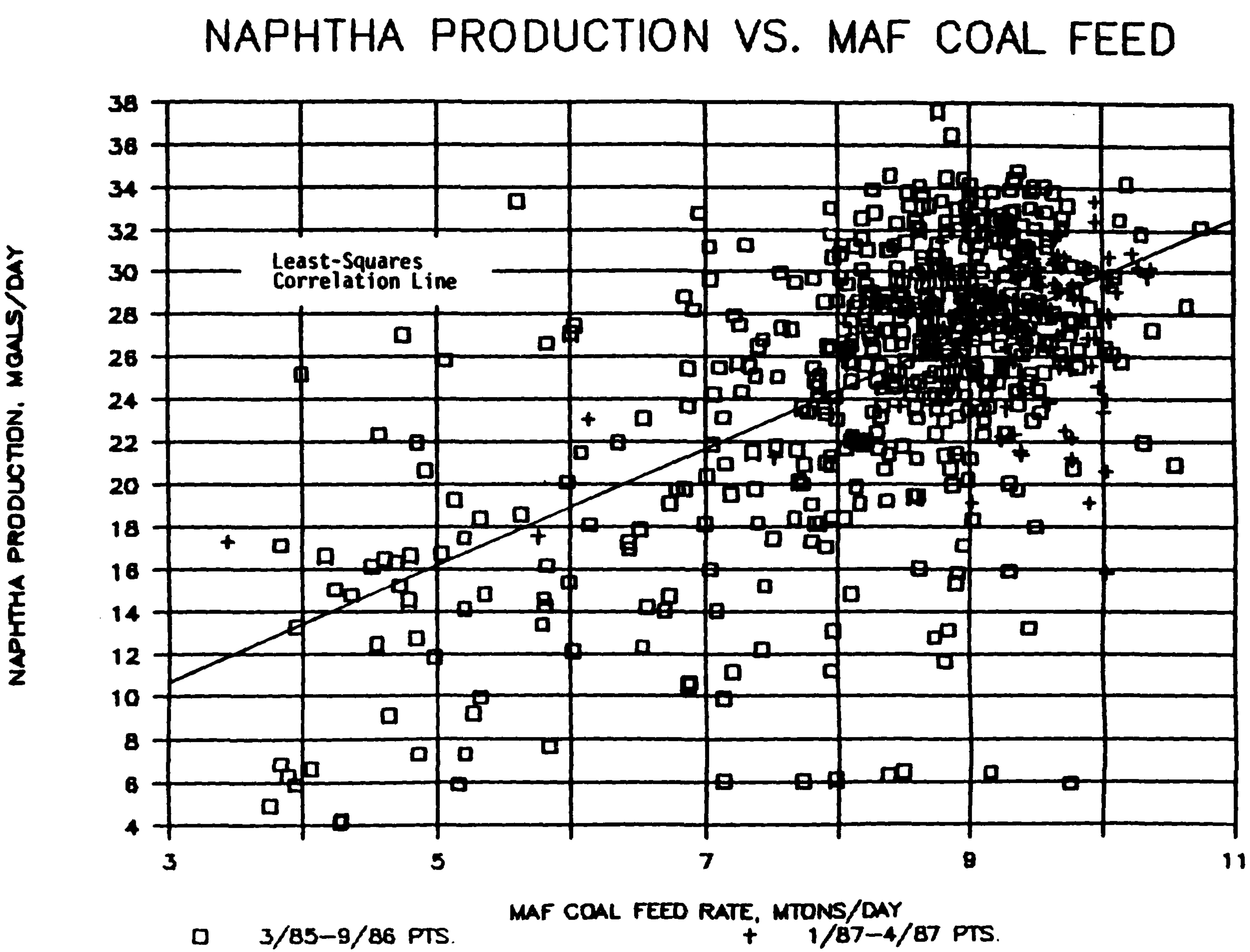

FIGURE 6. Naphtha Production vs. Maf Coal Feed Rate--Combined Large Data Base

were used to calculate a correlation of naphtha production as a function of maf coal feed rate. The parameters of the calculated correlation are shown in Table 1, and the detailed characteristics are shown in Table A-11 in the appendix. The correlation coefficient r is 0.60, which is highly significant statistically with 643 degrees of freedom. The correlation explains 36.0 percent of the sum of squares of deviations. The 1987 data are plotted in Figure 7, which also shows the correlation line.

6.3.4 Phenol Production. The two sets of phenol production data are plotted in Figure 8, and it can be seen that the two sets overlap to a considerable extent although the 1987 data may be somewhat lower on the average than the earlier data. The possible difference between the two sets was not judged to be significant enough to warrant the development of two separate correlations. Consequently, all of the data in both sets were used to calculate a correlation of phenol production as a function of maf coal feed rate. The parameters of the calculated correlation are shown in Table 1, and the detailed characteristics are shown in A-12 in the appendix. The correlation coefficient r is 0.53, which is slightly lower than that for the naphtha production correlation but still highly significant statistically. The 1987 data are plotted in Figure 9, which also shows the correlation line.

6.4 Correlations with Two Independent Variables

The combined small data base was used to develop improved correlations for tar oil production and phenol production by including the feed coal atomic H/C ratio as an additional correlating variable along with the maf coal feed rate. This effort was an extension of the earlier work described above in 5.4.

NAPHTHA PRODUCTION VS. MAF COAL FEED

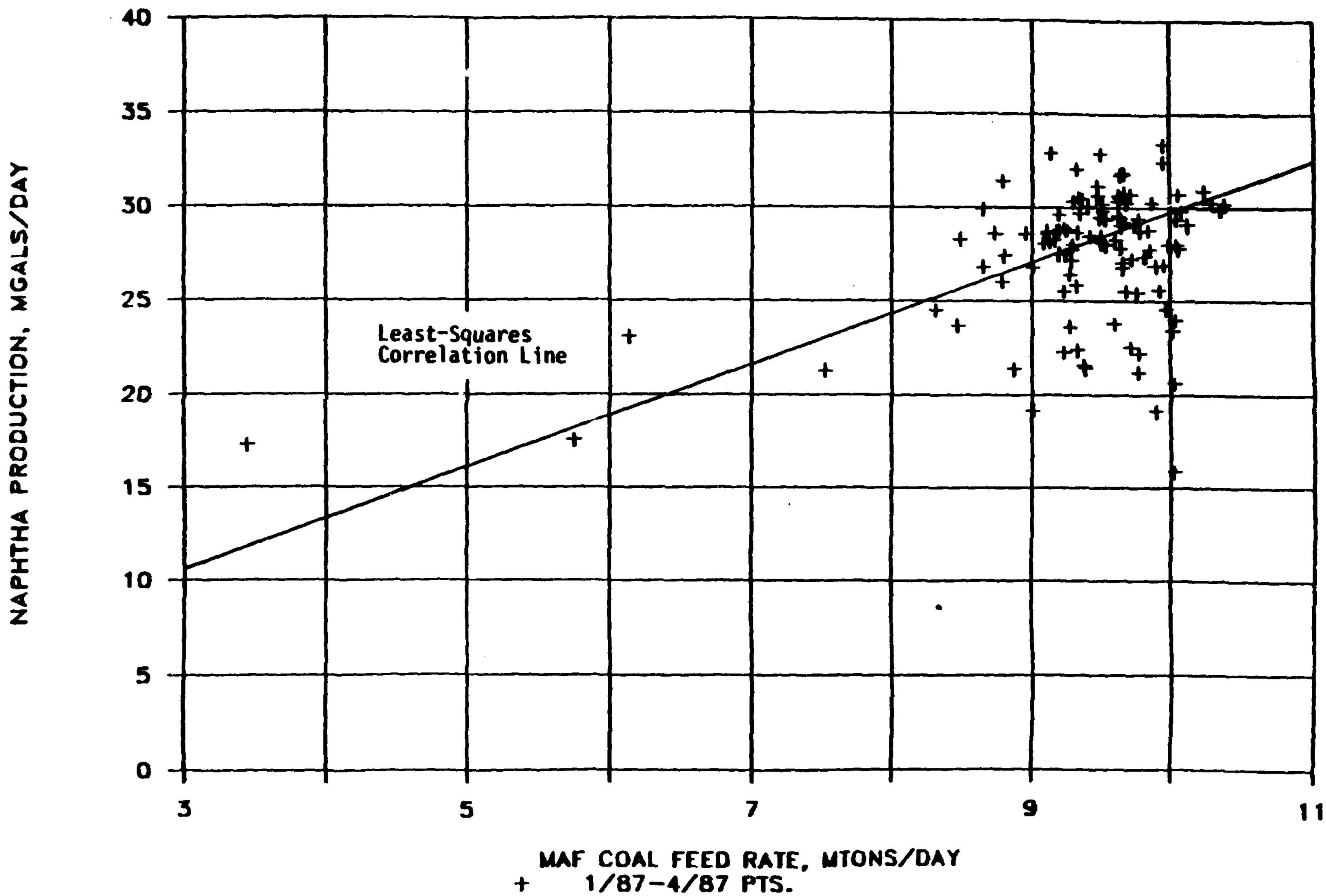

FIGURE 7. Naphtha Production vs. Maf Coal Feed Rate--1987 Data

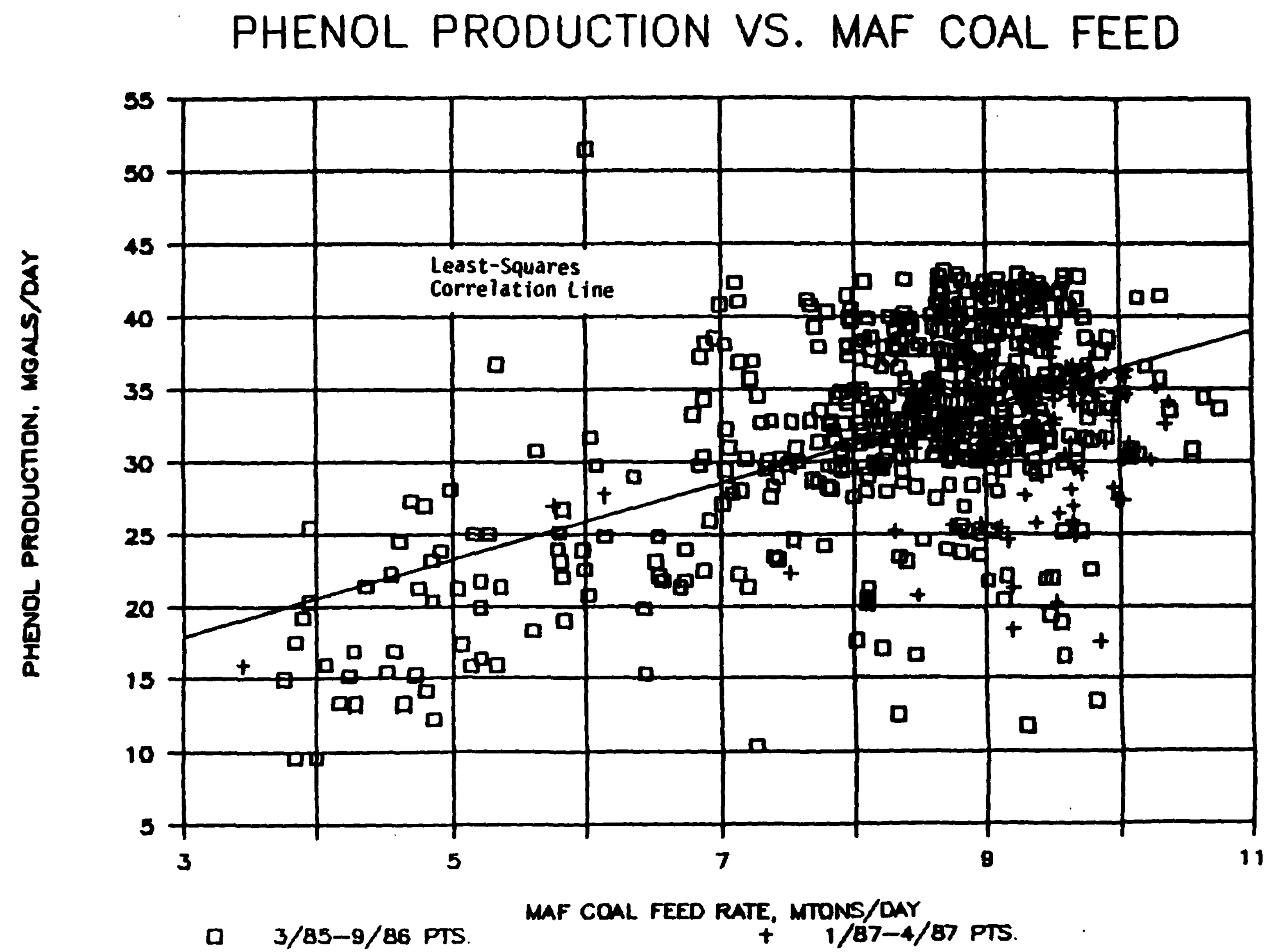

FIGURE 8. Phenol Production vs. Maf Coal Feed Rate--Combined Large Data Base

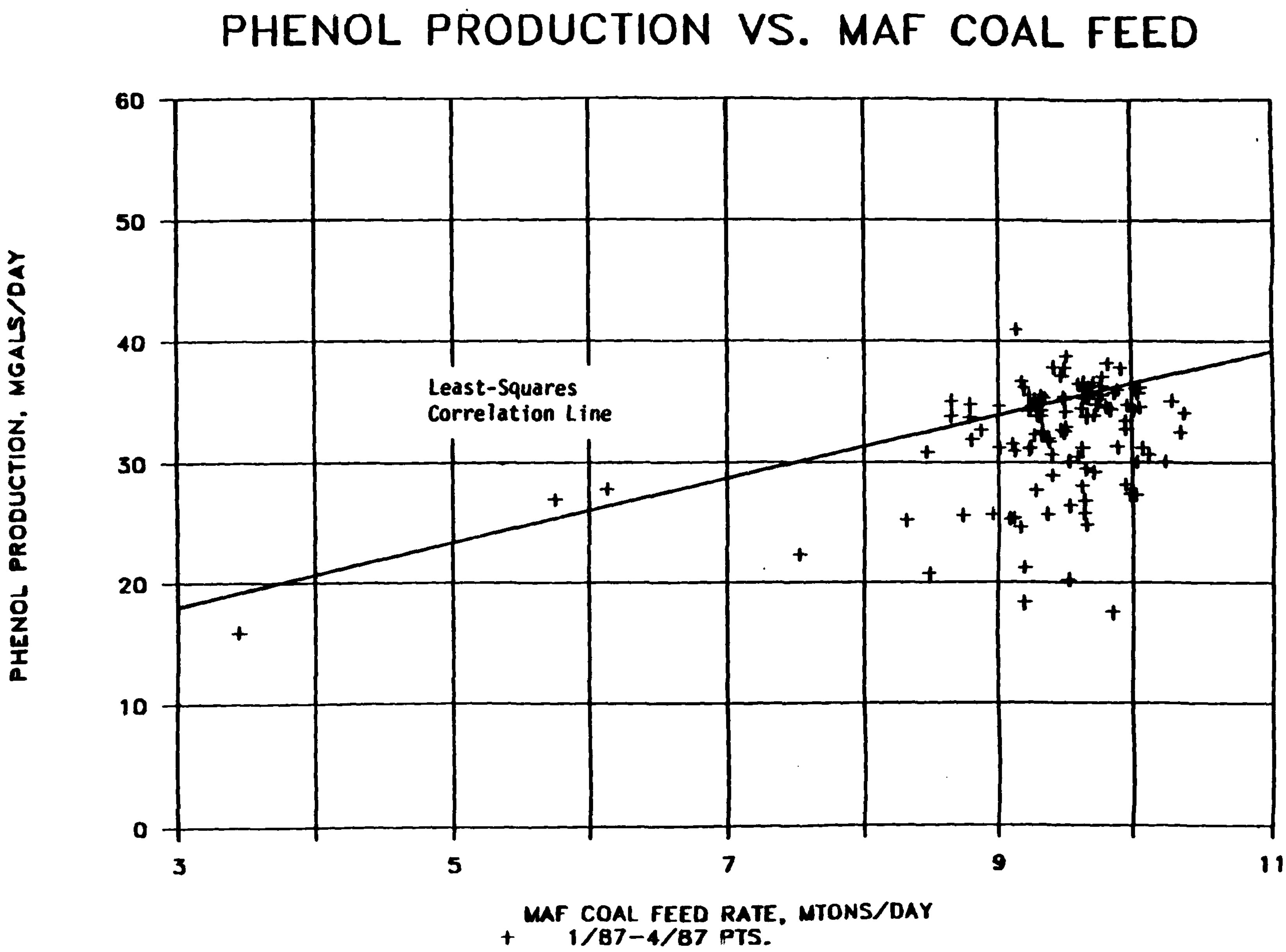

FIGURE 9. Phenol Production vs. Maf Coal Feed Rate--1987 Data

Table 3 lists the important parameters of the by-product correlations which include the atomic H/C ratio as a correlating variable. The characteristics of the data used for the correlations are shown in Table 4.

6.4.1 <u>Tar Oil Production.</u> The parameters of the calculated correlation of tar oil production with coal (maf) feed rate and atomic H/C ratio are shown in Table 3, and the detailed characteristics are shown in Table A-13 in the appendix. This correlation removes 32.1 percent of the sum of squares of deviations, and the correlation coefficient is 0.57. The extent of the improvement in the correlation by including H/C ratio as a second correlating variable can be seen by comparing these measures with those for a correlation with only coal (maf) feed rate (calculated from the same data base): 21.7 percent and 0.47, respectively. This correlation of tar oil production with coal (maf) feed rate and atomic H/C ratio is plotted in Figure 10 along with the data points for the combined small data base.

A plot of the tar oil production per ton of coal is shown in Figure 11, which shows that the tar oil produced per ton of feed coal decreases as the atomic H/C ratio of the feed coal increases. The parameters of this correlation are shown in Tables 2 and 3, and its characteristics in Table A-14 in the appendix.

For estimating the tar oil production for a given combination of maf coal feed rate and atomic H/C ratio, either correlation described above could be used. However, the correlation based on maf coal feed rate and H/C ratio, as opposed to estimating the tar oil production per ton, gives a slightly better estimate.

Table 3. Parameters of Final Correlations of Plant Products with Two Independent Variables

Number of points = 190 (combined data base) $\hat{y} = a + b_1x_1 + b_2x_2$

	1	2	3	4
Dependent variable y	tar oil Mgal/day	tar oil/maf coal gal/ton	phenol Mgal/day	phenol/maf coal gal/ton
Independent variable x_1	maf coal Mtons/day	atomic H/C	maf coal Mtons/day	atomic H/C
Independent variable x_2	atomic H/C		atomic H/C	
Intercept a	101.640	22.6722	4.03857	3.18817
Slope b_1	9.84191	-10.4802	2.63494	0.896637
Slope b_2	-80.0306		8.44477	
Sum of Squares Removed by Correlation	31314.7	177.9764	2117.97	1.30270
r^2	0.3208	0.1520	0.2798	0.0161

Table 4. Characteristics of Data Used for Final Correlation (Tables 2 and 3)

Number of points = 190 (combined data base)

Variable	Average	Minimum	Maximum	Sum of Squares of Deviations $\Sigma(y-\bar{y})^2$ or $\Sigma(x-\bar{x})^2$
Dependent:				
Tar Oil, Mgal/day	123.453	48.006	185.898	97615.3
Tar Oil/maf coal, gal/ton	14.382	9.555	22.398	1170.57
Phenol, Mgal/day	33.509	13.33	42.88	7568.87
Phenol/maf coal, gal/ton	3.897	1.784	5.945	81.1554
Independent:				
Maf coal, Mton/day	8.6490	3.444	10.5521	267.980
Atomic H/C	0.7911	0.5823	1.0749	1.6204

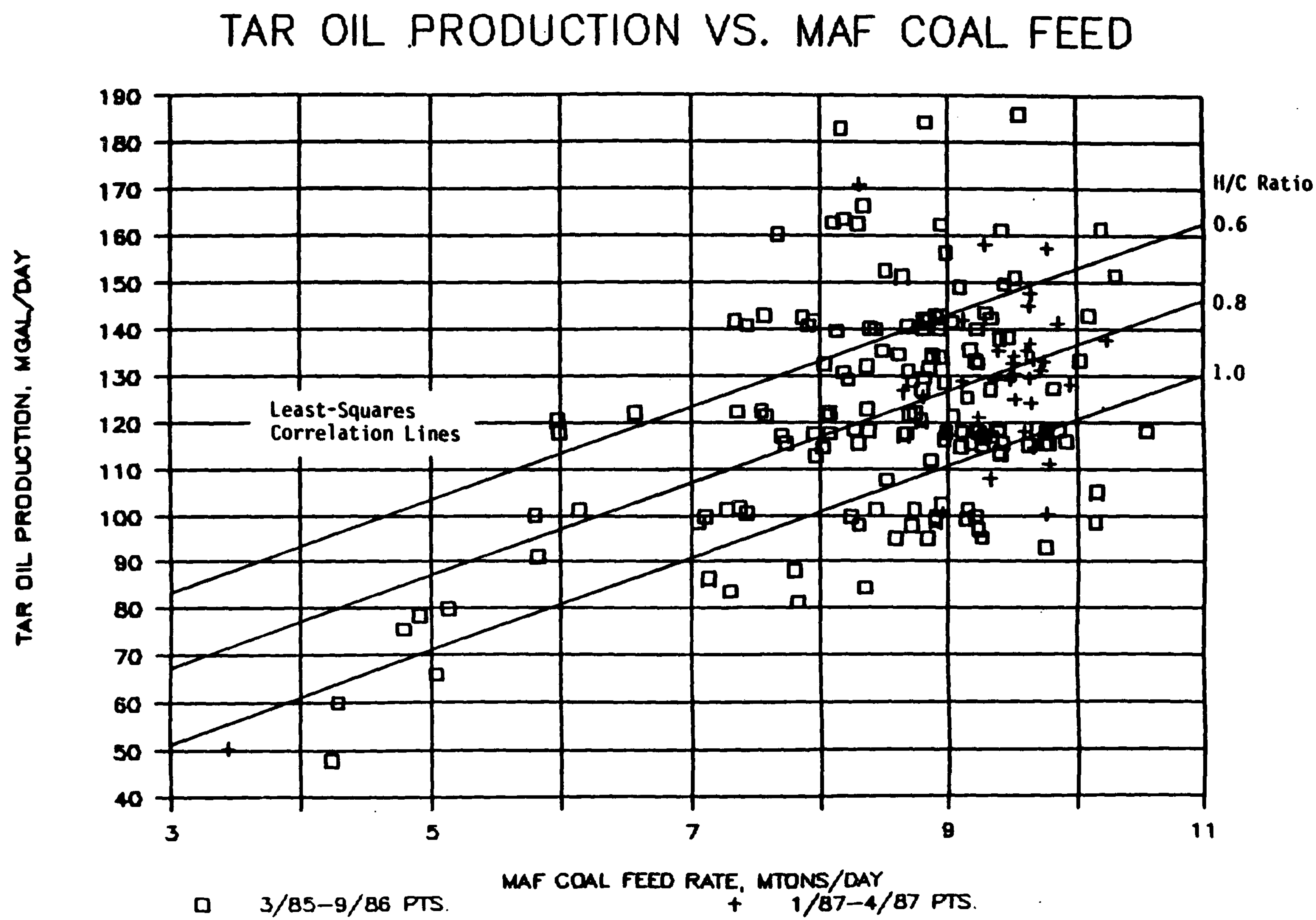

FIGURE 10. Tar Oil Production vs. Maf Coal Feed Rate--Combined Small Data Base

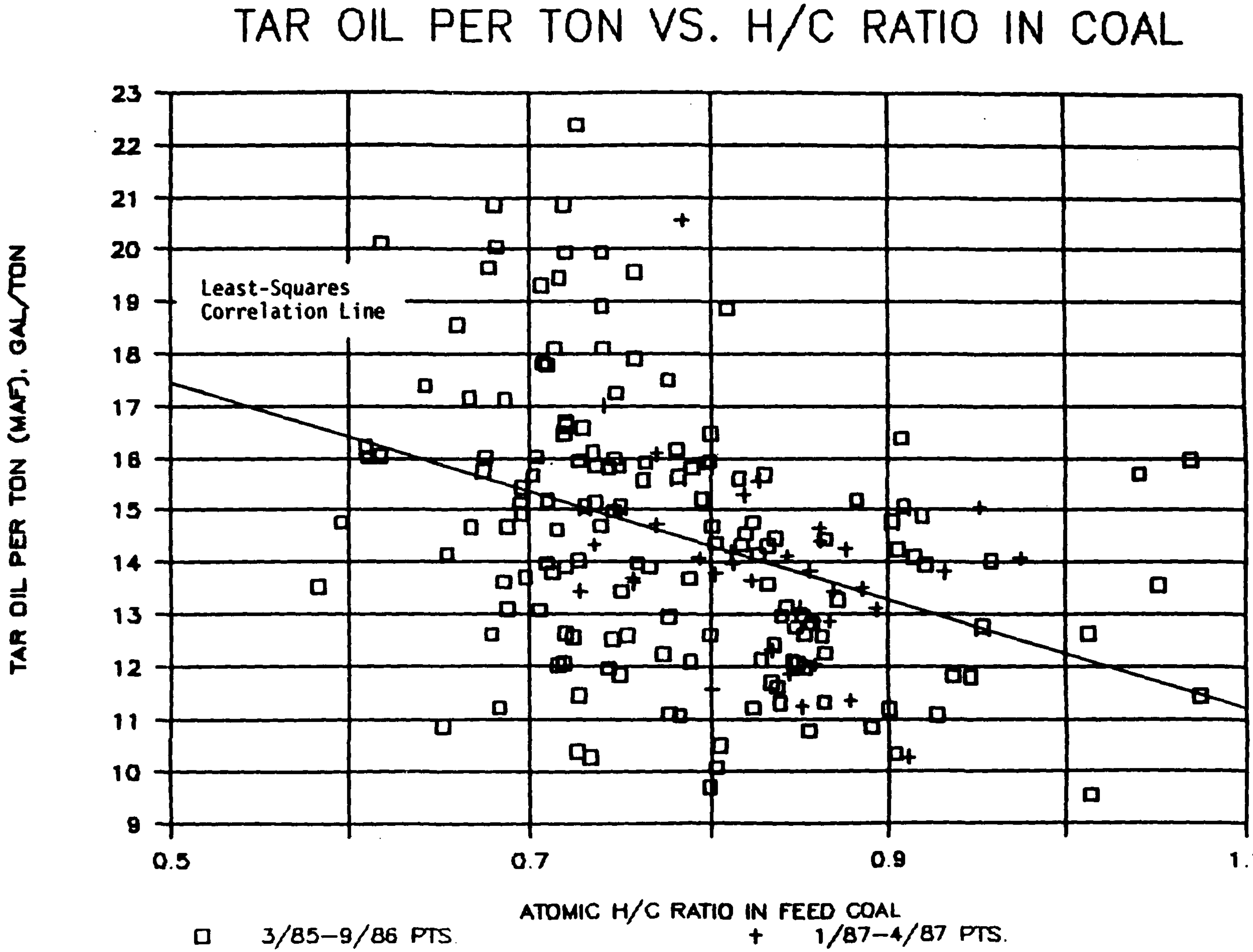

FIGURE 11. Tar Oil Per Ton vs. Atomic H/C Ratio--Combined Small Data Base

6.4.2 <u>Phenol Production.</u> The parameters of the calculated correlation of phenol production with coal (maf) feed rate and atomic H/C ratio are shown in Tables 2 and 3, and the detailed characteristics are shown in Table A-15 in the appendix. This correlation removes 28.0 percent of the sum of squares of deviations, and the correlation coefficient is 0.53. The extent of the improvement in the correlation by including the H/C ratio as a second correlating variable can be seen by comparing these measures with those for a correlation with only coal (maf) feed rate (calculated from the same data base): 26.5 percent and 0.51 respectively. This correlation of phenol production with coal (maf) feed rate and atomic H/C ratio is plotted in Figure 12, along with the data points for the combined small data base.

A plot of the phenol production per ton of coal is shown in Figure 13, which shows that the phenol produced per ton of feed coal may increase somewhat as the atomic H/C ratio of the feed coal increases. The parameters of the correlation are shown in Table 3, and the correlation is plotted in Figure 13. In addition of the 1987 phenol data, which tend to be low compared to the 1985-1986 data, to the data base had the effect of making this correlation less certain than the correlation calculated from only the 1985-1986 data. The correlation for pnenol production as a function of coal (maf) feed rate and atomic H/C ratio gives a better estimate than the correlation for phenol production per ton.

7.0 DISCUSSION OF RESULTS

Although the product correlations resulting from this effort do not include the effects of gasifier operating conditions, the results do provide some insight into the formation of the by-products. The

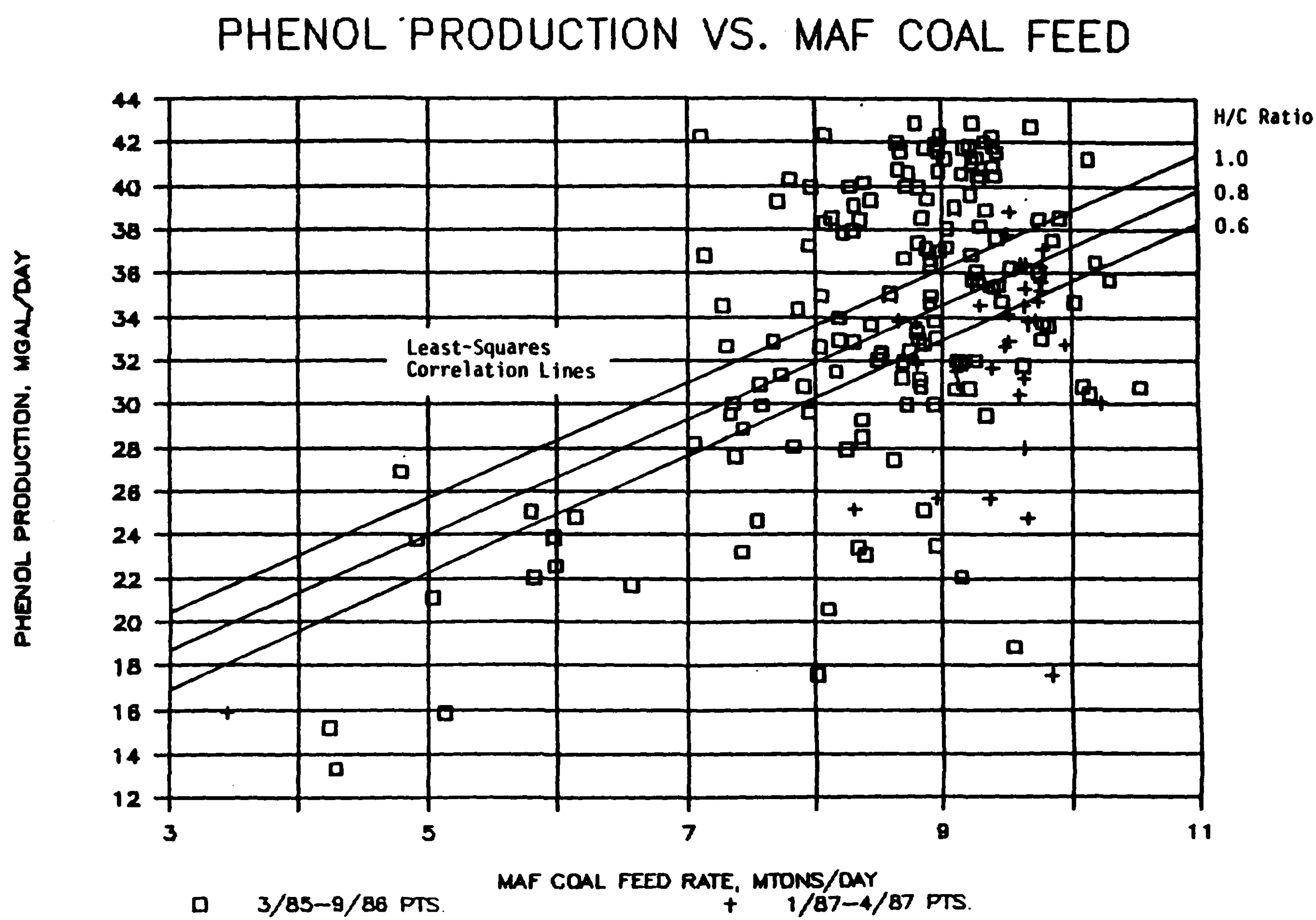

FIGURE 12. Phenol Production vs. Maf Coal Feed Rate--Combined Small Data Base

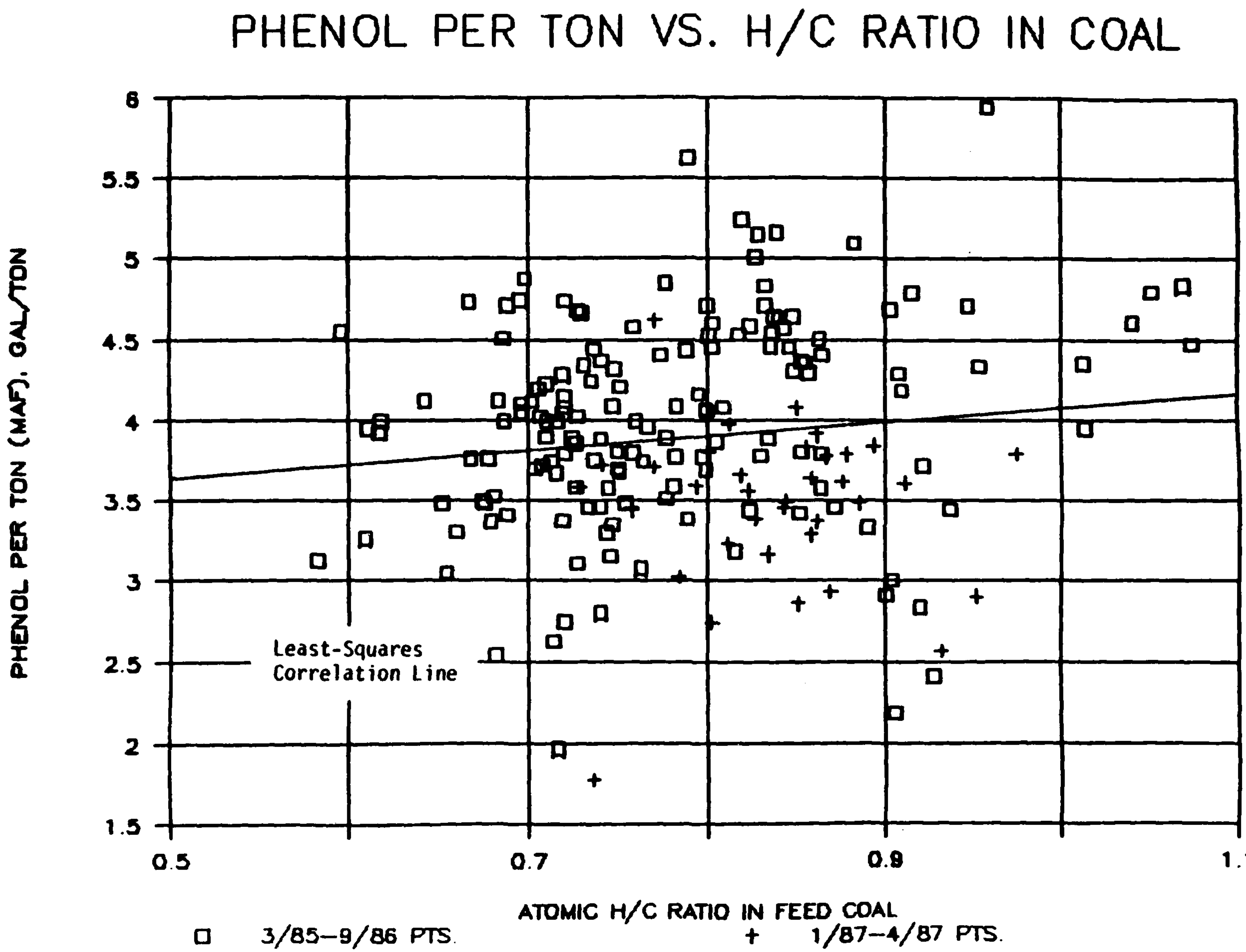

FIGURE 13. Phenol Per Ton vs. Atomic H/C Ratio--Combined Small Data Base

results illustrate the variability of the plant production of the various products, although it is not possible to explain all of the variability in production on the basis of the available data on potential influential variables. The correlations for the various products may be used to estimate the average amount of production for any given set of conditions. The variability of the estimate is also described, in terms of a standard deviation and confidence limits. The following sections summarize the discussion of correlation results with respect to key variables.

- The amount of SNG production is largely determined by the maf coal feed rate. Over 80 percent of the sum of squares of deviations was explained by this one variable. SNG production did not seem to be affected by any of a number of feed coal characteristics including percent volatile matter, ash, Na_2O content, ash fusion temperature, sulfur, or H/C ratio. SNG production perhaps should depend on residence time of the coal within the gasifiers, but this variable tends to be held fairly constant at the GPGP and thus should not be a significant factor in the present set of data. The lack of influence of feed coal characteristics upon SNG production means that these parameters may be varied to influence the liquid by-product production without interfering with SNG.

- The tar oil production is most strongly controlled by the maf coal feed rate, although this one variable alone explains little more than 26 percent of the sum of squares of deviation. Tar oil production also appears to be a function of the atomic H/C ratio of the feed coal, decreasing with an increase in value of this coal characteristic. Tar oil production is also influenced by various operating parameters downstream of the gasifier for which there are no available data at this time.

- Production of phenol is influenced by the maf coal feed rate, and to some degree, the atomic H/C ratio. As this latter variable

increases, so may phenol production. The phenol stream is also a possible feedstock for jet fuel production.

- The fact that the tar oil and the phenol productions are functions of feed coal H/C ratio perhaps is an indication that the H/C ratio represents the types of volatiles contained in the coal. A higher H/C ratio indicates that the volatiles are somewhat lighter in composition and have more single-ring compounds, and vice-versa for a lower H/C ratio - the volatiles have more multi-ring compounds likely to wind up as tar oil.

- The percent volatile matter of the feed coal is an important parameter which influences the yield of liquid products resulting from coal pyrolysis. However, this parameter does not appear to play any role in determining the yields of liquid by-products in coal gasification. This is probably so because the pyrolytic reactions are not allowed to go to completion. Rather the devolatilization zone is comparatively small, and the coal travels very quickly into the gasification region.

- The yields of tar oil and phenols could probably be increased by any mechanism or pretreatment of the coal which would allow the volatiles to escape more easily or quickly, when the coal is fed into the gasifier. Particle size would be one such variable. The smaller the particle size, the more easily the volatiles can escape before the particle travels into the gasification zone. Of course, there are limits on the appropriate coal particle size which can be accommodated by the gasifier. However, it would be of interest to collect the data on particle size distribution and to try to relate this variable to tar oil and phenol production.

- The correlations for tar oil and phenol indicates that there is a tradeoff between the two by-products which can be made as a function of the atomic H/C ratio of the feed coal. A lower H/C ratio - for example, going from 0.8 to 0.7 - would increase tar oil by 1

gal/ton maf coal and lower phenol by 0.1 gal/ton. Since phenol is a more difficult compound to hydrotreat to get rid of the oxygen, the net result would be to increase jet fuel production and to decrease operating costs. On the other hand, the suggestion has been made to market the phenols. By-product credits could, therefore, be increased by using a feed coal with a high H/C ratio.

- The 1987 data on production do not appear to be significantly different from the 1985-1986 data.

8.0 CONCLUSIONS

The following conclusions summarize the findings developed from this initial effort to correlate the liquid by-product production data from the GPGP.

- For all four products analyzed - SNG, tar oil, naphtha, and phenol - the maf coal feed rate was the most influential independent variable.

- For SNG production the maf coal feed rate was the only influential independent variable. With this variable alone more than 80 percent of the sum of squares of deviations was removed - a very good correlation with 116 data points (1987 data only).

- No feed coal characteristic examined, including percent volatile matter, H/C ratio, percent sulfur, percent ash, percent Na_2O, or ash fusion temperature contributed very much to a better correlation for SNG production.

- Tar oil production was influenced most strongly by maf coal feed rate. Although the correlation removed only slightly more than 26 percent of the sum of squares of deviations, the correlation was still found to be significant because of the relatively large number of data points (645).

- Tar oil production was found to be influenced by the atomic H/C ratio of the feed coal, and a correlation was developed using both the maf coal feed rate and the atomic H/C ratio as correlating variables.

- Tar oil produced per ton of maf coal was found to decrease with increased H/C ratio.

- Tar oil production was not found to be influenced by percent volatile matter, percent sulfur, percent ash, percent Na_2O, or ash fusion temperature in the feed coal.

- To smooth out variations in tar oil production caused by the measuring method, three-day rolling averages were used to develop a correlation with maf coal feed rate, but the correlation was not very different from one calculated from the original daily data.

- A correlation was developed for naphtha production with maf coal feed rate as the correlating variable.

- A correlation was calculated for phenol production with both maf coal feed rate and atomic H/C ratio as correlating variables.

- Phenol production per ton was found to increase slightly with increased H/C ratio of the feed coal.

- This analysis and the correlations that were developed describe the variability of the plant production of the various products, although it is not currently possible to explain all of the variability in production on the basis of the available data.

- Theories of coal devolatilization and pyrolysis can help explain the formation of the liquid by-products in gasification, although more analysis along this line of investigation is required.

- The 1987 data on production do not appear to be significantly different from the 1985-1986 data.

9.0 RECOMMENDATIONS

As the result of this initial effort to analyze the data on liquid by-product production at the GPGP, the following recommendations are made to develop the data correlations further and to make use of the correlations in the jet fuel production program.

- Further study and analysis of the basic processes occurring in the gasifier to produce the liquid by-products should be done. With this information a model for their formation can be developed, and the important parameters controlling their production can be identified and incorporated into the data correlations.

- An analysis should be made of the operations occurring after the gasifier that affect the quality and quantity of the liquid by-products. Important parameters affecting by-product production can be identified for collecting data for later incorporation into the correlations.

- Composition data on the tar oil should be analyzed and compared to feed coal composition data and operating data to learn more about tar oil formation in the gasifier and feedstock characteristics.

- An effort should be made to obtain gasifier operating data, on a restricted basis if necessary, to incorporate such parameters as the steam rate, temperature, and pressure into the correlations.

- The correlations that have been developed should be used in technical and economic tradeoff studies to estimate tar oil and phenol production versus feed coal characteristics to develop the optimum design for the jet fuel production facilities.

- Since the correlations have identified atomic H/C ratio as an important feed coal characteristic affecting liquid by-product productions, data should be gathered on feed coal characteristics and supply sources to identify and quantify potential feed coals for producing jet fuel feedstocks.

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APPENDIX

Table A-1. Preliminary Correlations of Tar Oil Production in GPGP

1985-1986 Data

Tar oil production, gal/day $\hat{y} = a + b_1 x_1 + b_2 x_2$
Number of points = 535 Sum of squares of y $[\Sigma(y-\bar{y})^2]$ = 313,185,000,000

Correlation No.	Independent Variable x_1	Independent Variable x_2	Intercept a	Slope b_1	Slope b_2	Sum of Squares Removed by Correlation ($\times 10^6$)
1	SNG production MMSCF/day	--	61,168.	461.14	--	75,239
2	maf coal feed rate tons/day	--	46,500.	8.7997	--	79,941
3	"	SNG production MMSCF/day	48,708.	5.9732	168.12	81,693
4	"	% sulfur (maf)	42,515.	8.8725	3670.2	80,585
5	"	% ash (maf)	41,125.	8.9432	426.16	80,613

Table A-2. Characrteristics of Data Used for Preliminary Tar Oil Production Correlations (Table A-1)

1985-1986 Data

Variable	Number of Points	Average	Minimum	Maximum
1. Tar oil production, gal/day	535	118,883	14,116	200,698
2. SNG production, MMSCF/day	535	125.16	8.66	156.33
3. Maf coal feed rate, tons/day	535	8,225.7	3,726.7	10,757.2
4. % sulfur (maf)	535	0.9227	0.34	2.30
5. % ash (maf)	535	9.840	5.1	28.4

Table A-3. Preliminary Correlations with One Independent Variable to Identify Important Variables 1985-1986 Data

Number of points = 157 $\hat{y} = a + b\,x$

Correlation No.	Dependent Variable y	Independent Variable x	Intercept a	Slope b	Removed by Correlation	r^2
1	SNG production,MMSCF/day	Maf coal feed,tons/day	-13.2316	0.0168081	67,150.4	0.8119
2	"	% volatile matter	144.715	-0.329288	16.3037	0.0002
3	"	Atomic H/C ratio	115.057	17.4984	432.060	0.0052
4	"	Volatile matter,tons/day	-8.94540	0.0335384	64,991.4	0.7858
5	"	No. gasifiers	-26.0115	12.2903	16,689.8	0.2018
6	Tar oil production,gal/day	MAF coal feed,tons/day	42,667.9	9.30354	20,573,300,000	0.2115
7	"	% volatile matter	27,751.1	1923.89	556,535,000	0.0057
8	"	Atomic H/C ratio	176,313.0	-70,562.5	7,025,770,000	0.0722
9	"	Volatile matter,tons/day	43,070.8	19.0463	20,960,000,000	0.2155
10	"	No. gasifiers	-15,238.7	10,841.4	12,986,800,000	0.1335
11	Naphtha production,Mgal/day	MAF coal feed,tons/day	2.37148	0.00271958	1757.97	0.2684
12	"	% volatile matter	24.7217	0.0126872	0.0242026	0.0000
13	"	Atomic H/C ratio	22.2297	3.98332	22.3891	0.0034
14	"	Volatile matter,tons/day	3.01646	0.00543838	1708.87	0.2609
15	"	No. gasifiers	17.8972	0.591071	38.6019	0.0059
16	Phenol production, Mgal/day	MAF coal feed,tons/day	9.34746	0.00290729	2009.03	0.2842
17	"	% volatile matter	70.7664	-0.758625	86.5343	0.0122
18	"	Atomic H/C ratio	21.0063	16.5213	385.153	0.0545
19	"	Volatile matter,tons/day	10.8395	0.00561823	1823.77	0.2580
20	"	No. gasifiers	20.9925	1.02524	116.140	0.0164

Table A-4. Characteristics of Data Used for Preliminary Correlations (Table A-3)

1985-1986 Data

157 points

Variable	Average	Minimum	Maximum	$\Sigma(y-\bar{y})^2$
Dependent:				
SNG, MMSF/day	128.713	18.380	156.326	82,703.7119
Tar oil, gal/day	121,246.20	14,264	185,898	97,262,297,000
Naphtha, Mgal/day	25.3383	4.22	36.50	6550.2004
Phenol, Mgal/day	33.8995	13.33	51.45	7069.8711
Independent:				
Maf coal, tons/day	8444.99	3886.09	10,552.09	
% volatile matter	48.5970	44.64	52.52	
Atomic H/C	0.7804	0.5823	1.0749	
Volatile matter, tons/day	4104.50	1900.30	5062.19	
Avg. No. Gasifiers	12.5892	8.6	14.0	

Table A-5. Parameters of Initial Correlations of Plant Products versus the Maf Coal Feed Rate

1985-1986 Data

Number of points = 529 $\hat{y} = a + b\ x$

Dependent Variable y	Independent Variable x	Intercept a	Slope b	Initial Sum of Squares $\sum(y-\bar{y})^2$	Sum of Squares Removed	r^2
SNG production, MMSCFD	maf coal feed rate, tons/day	-12.8888	0.0167844	334,334	272,609	0.8154
Tar oil production, gal/day	"	48,773.4	8.54084	3.02433×10^{11}	7.05879×10^{10}	0.2334
Naphtha production, M gal/day	"	1.13112	0.00288794	22,343.8	8070.57	0.3612
Phenol production, M gal/day	"	7.53771	0.00299797	26,096.7	8697.30	0.3333

Table A-6. Characteristics of Data Used for Initial Correlations (Table A-5)

1985-1986 Data

529 points

Variable	Average	Minimum	Maximum	$\sum(y-\bar{y})^2$
Dependent:				
SNG, MMSCF/day	125.77297	8.66	156.326	334,334
Tar oil, gal/day	119,332.243	14,116	200,698	3.02433×10^{11}
Naphtha, Mgal/day	24.98935	4.16	37.6	22,343.8
Phenol, Mgal/day	32.3050	9.66	51.45	26,096.7
Independent:				
Maf coal, tons/day	8261.3439	3754.0875	10,757.1789	

Table A-7. Correlations with Two Independent Variables

1985-1986 Data

Number of points = 154

$$\hat{y} = a + b_1x_1 + b_2x_2$$

	1	2	3	4	5
Dependent Variable y	tar oil gal/day	tar oil/maf coal gal/ton	tar oil/maf coal gal/ton	phenol Mgal/day	phenol/maf coal gal/ton
Independent Variable x_1	maf coal tons/day	Atomic H/C	Atomic H/C	maf coal tons/day	Atomic H/C
Independent Variable x_2	Atomic H/C	---	$(\text{Atomic H/C})^2$	Atomic H/C	---
Intercept a	108,594	22.6504	37.0095	-2.82746	2.72739
Slope b_1	9.21652	-10.4270	-46.1949	0.00311841	1.62802
Slope b_2	-82,683.0	---	21.9266	13.0516	---
Sum of Squares Removed by Correlation	25,185,100,000	153.235	166.051	2390.82	3.73561
r^2	0.3037	0.1468	0.1591	0.3658	0.0581

Table A-8. Characteristics of Data Used for Correlations (Table A-7)

1985-1986 Data

154 points

Variable	Average	Minimum	Maximum	$\sum(y-\bar{y})^2$
Dependent:				
Tar oil, gal/day	122,377.7	48,006	185,898	82,939,600,000
Tar oil/maf coal, gal/ton	14.5113	9.5545	22.3976	1043.73
Phenol, Mgal/day	33.8615	13.3300	42.8800	6536.22
Phenol/maf coal, gal/ton	3.998189	1.972576	5.945286	64.2763
Independent:				
Maf coal, tons/day	8498.29	4241.15	10,552.09	
Atomic H/C	0.780580	0.582322	1.074916	
$(H/C)^2$	0.618457	0.339099	1.155444	

Table A-9. Characteristics of the Correlation of SNG Production vs. Coal (maf) Feed Rate--1987 Data

Estimated SNG production (quantity billed plus internal consumption), MMSCF/day, for a particular coal (maf) feed rate, M tons/day: $\hat{y} = 5.31437 + 15.0912\,x$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{18975.2}{23489.2} = 0.8078$$

correlation coefficient, $r = 0.90$
variance of average y, $s^2(\bar{y}) = 0.3414$
standard deviation of average y, $s(\bar{y}) = 0.58$

variance of slope, $s^2(b) = 0.4752$
standard deviation of slope, $s(b) = 0.69$

variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.3414 + 0.4752\,(9.380 - x_i)^2$$

standard deviation of any average estimated value, $\hat{y}_i$: $S(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96\sqrt{0.3414 + 0.4752\,(9.380 - x_i)^2}$$

Table A-10. Characteristics of the Correlation of Tar Oil Production vs. Coal (maf) Feed Rate--Combined Large Data Base

Estimated tar oil production, M gal/day,
for a particular coal (maf) feed rate, M tons/day: $\hat{y} = 46.5664 + 8.89910\ x$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{92659.9}{351849.7} = 0.2634$$

correlation coefficient, $r = 0.51$
variance of average y , $s^2\ (\bar{y}) = 0.6250$
standard deviation of average y , $s(\bar{y}) = 0.79$

variance of slope, $s^2(b) = 0.3445$
standard deviation of slope, $s(b) = 0.59$

variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.6250 + 0.3445\ (8.463 - x_i)^2$$

standard deviation of any average estimated value, $\hat{y}_i$: $S(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96 \sqrt{0.6250 + 0.3445\ (8.463 - x_i)^2}$$

Table A-11. Characteristics of the Correlation of Naphtha Production vs. Coal (maf) Feed Rate--Combined Large Data Base

Estimated naphtha production, M gal/day,
for a particular coal (maf) feed rate, M tons/day: $\hat{y} = 2.26738 + 2.73966\ x$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{8781.99}{24402.8} = 0.3599$$

correlation coefficient, $r = 0.60$
variance of average y , $s^2\ (\bar{y}) = 0.0377$
standard deviation of average y , $s(\bar{y}) = 0.19$

variance of slope, $s^2(b) = 0.0208$
standard deviation of slope, $s(b) = 0.14$

variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.0377 + 0.0208\ (8.463-x_i)^2$$

standard deviation of any average estimated value, $\hat{y}_i$: $S(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96 \sqrt{0.0377 + 0.0208\ (8.463-x_i)^2}$$

Table A-12. Characteristics of the Correlation of Phenol Production vs. Coal (maf) Feed Rate--Combined Large Data Base

Estimated phenol production, M gal/day, for a particular coal (maf) feed rate, M tons/day: $\hat{y} = 10.0519 + 2.62406\ x$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{8056.56}{28761.9} = 0.2801$$

correlation coefficient, $r = 0.53$
variance of average y, $s^2\ (\bar{y}) = 0.0499$
standard deviation of average y, $s(\bar{y}) = 0.22$

variance of slope, $s^2(b) = 0.0275$
standard deviation of slope, $s(b) = 0.17$

variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.0499 + 0.0275\ (8.463-x_i)^2$$

standard deviation of any average estimated value, $\hat{y}_i$: $s(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96\sqrt{0.0499 + 0.0275\ (8.463-x_i)^2}$$

Table A-13. Characteristics of the Correlation of Tar Oil Production--Combined Small Data Base

Estimated tar oil production, M gal/day, for a particular coal (maf) feed rate, x_1, M *tons/day*, and atomic H/C ratio, x_2: $\hat{y} = 101.640 + 9.84191\, x_1 - 80.0306 x_2$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{31314.7}{97615.3} = 0.3208$$

correlation coefficient, $r = 0.57$
variance of average y , $s^2\,(\bar{y}) = 1.8660$
standard deviation of average y , $s(\bar{y}) = 1.37$
variance of slope b_1, $s^2(b_1) = 1.3547$
standard deviation of slope, b_1, $s(b_1) = 1.16$
variance of slope b_2, $s^2(b_2) = 224.05$
standard deviation of slope, b_2, $s(b_2) = 14.97$
variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 1.8660 + 1.3547(x_{1i}-8.649)^2 + 224.05(x_{2i} - 0.7911)^2 + 5.3296(x_{1i}-8.649)(x_{2i}-0.7911)$$

standard deviation of any average estimated value, $\hat{y}_i$: $s(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96 \sqrt{1.8660 + 1\,.\,3547(x_{1i}-8.649)^2 + 224.05(x_{2i} - 0.7911)^2 + 5.3296(x_{1i}-8.649)(x_{2i}-0.7911)}$$

Table A-14. Characteristics of the Correlation of Tar Oil Production Per Ton vs. Atomic H/C Ratio--Combined Small Data Base

Estimated tar oil production per ton, gal/ton, for a particular atomic H/C ratio: $\hat{y} = 22.6722 - 10.4802\ x$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{177.976}{1170.57} = 0.1520$$

correlation coefficient, $r = 0.39$
variance of average y , $s^2\ (\bar{y}) = 0.0278$
standard deviation of average y , $s(\bar{y}) = 0.17$

variance of slope, $s^2(b) = 3.2583$
standard deviation of slope, $s(b) = 1.81$

variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.0278 + 3.2583(0.7911 - x_i)^2$$

standard deviation of any average estimated value, $\hat{y}_i$: $s(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96\sqrt{0.0278 + 3.2583(0.7911 - x_i)^2}$$

Table A-15. Characteristics of the Correlation of Phenol Production--Combined Small Data Base

Estimated phenol production, M gal/day,
for a particular coal (maf) feed rate, x_1, M tons/day,
and atomic H/C ratio, x_2: $\hat{y} = -4.03857 + 2.63494\, x_1 + 8.44477\, x_2$

ratio of sum of squares removed to original sum of squares, r^2:

$$r^2 = \frac{2117.97}{7568.87} = 0.2798$$

correlation coefficient, $r = 0.53$
variance of average y, $s^2(\bar{y}) = 0.1534$
standard deviation of average y, $s(\bar{y}) = 0.39$
variance of slope b_1, $s^2(b_1) = 0.1114$
standard deviation of slope b_1, $s(b_1) = 0.33$
variance of slope, b_2, $s^2(b_2) = 18.4197$
standard deviation of slope b_2, $s(b_2) = 4.29$
variance of any average estimated value, $\hat{y}_i$:

$$s^2(\hat{y}_i) = 0.1534 + 0.1114(x_{1i}-8.6490)^2 + 18.4197(x_{2i}-0.7911)^2 + 0.4382(x_{1i}-8.6490)(x_{2i}-0.7911)$$

standard deviation of any average estimated value, $\hat{y}_i$: $s(\hat{y}_i)$

confidence limits (95%) of any average estimated value, $\hat{y}_i$:

$$y_i = \hat{y}_i \pm 1.96\sqrt{0.1534 + 0.1114(x_{1i}-8.6490)^2 + 18.4197(x_{2i}-0.7911)^2 + 0.4382(x_{1i}-8.6490)(x_{2i}-0.7911)}$$

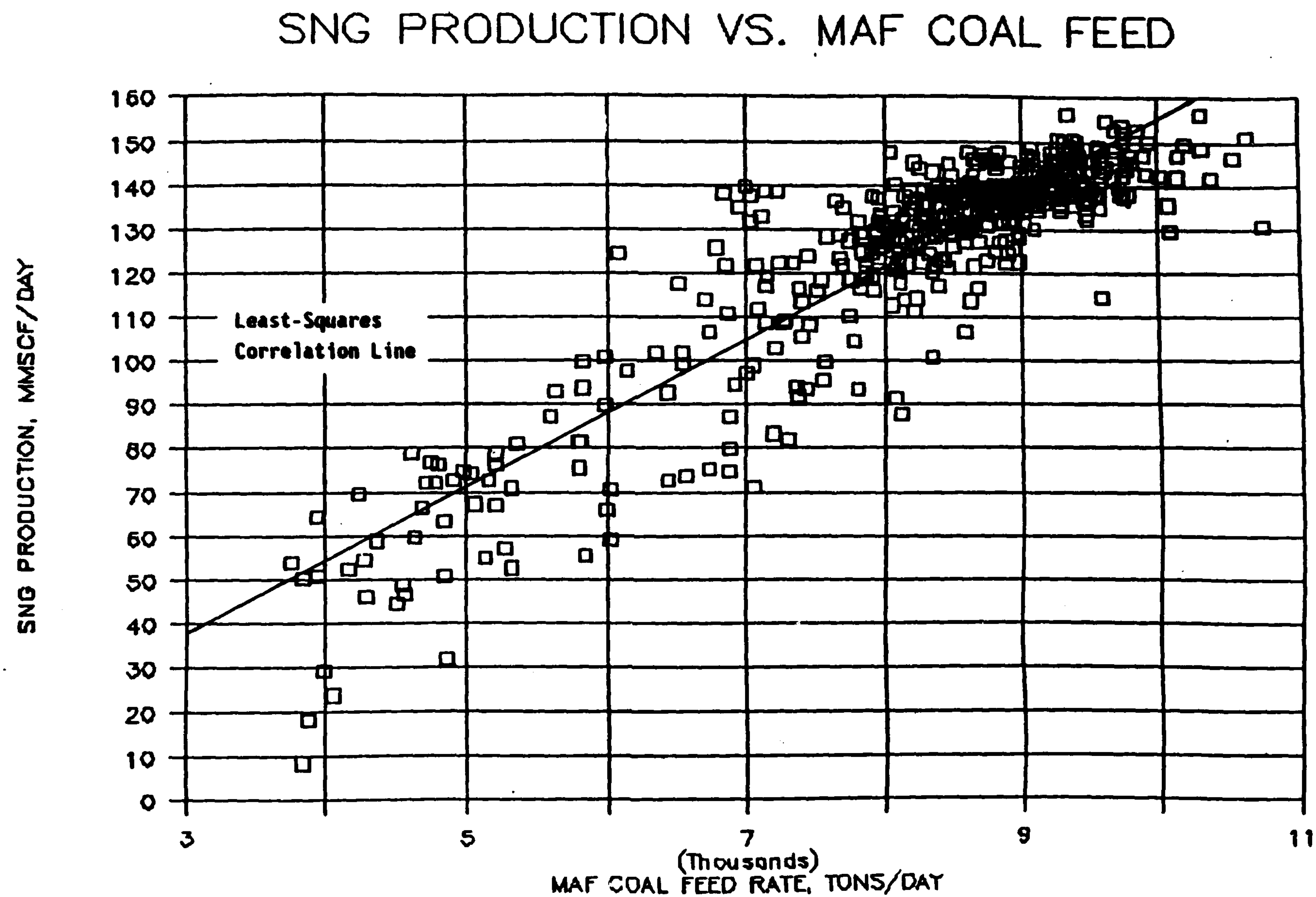

FIGURE A-1. SNG Production vs. Maf Coal Feed--1985-1986 Data

TAR OIL PRODUCTION VS. MAF COAL FEED

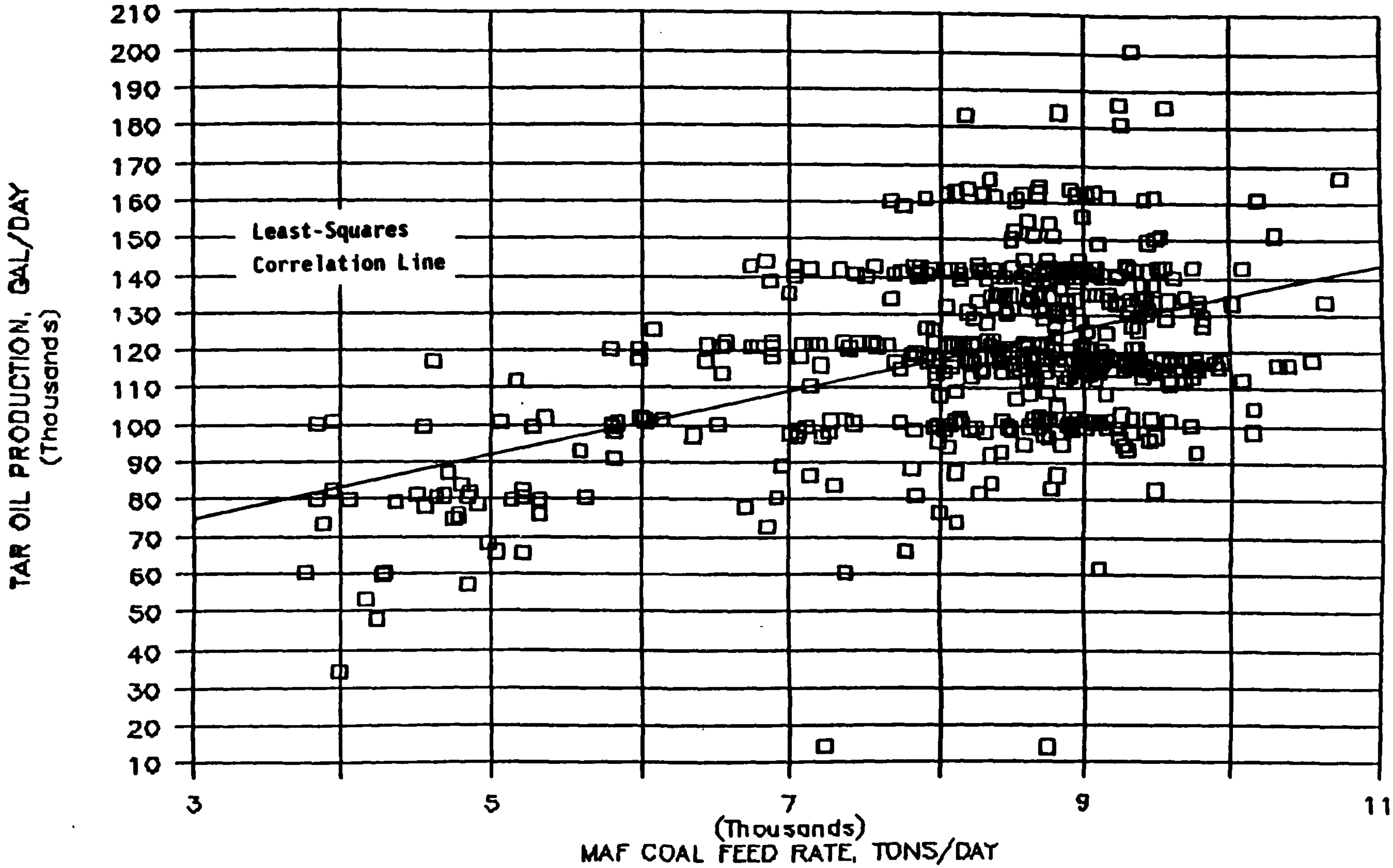

FIGURE A-2. Tar Oil Production vs. Maf Coal Feed--1985-1986 Data

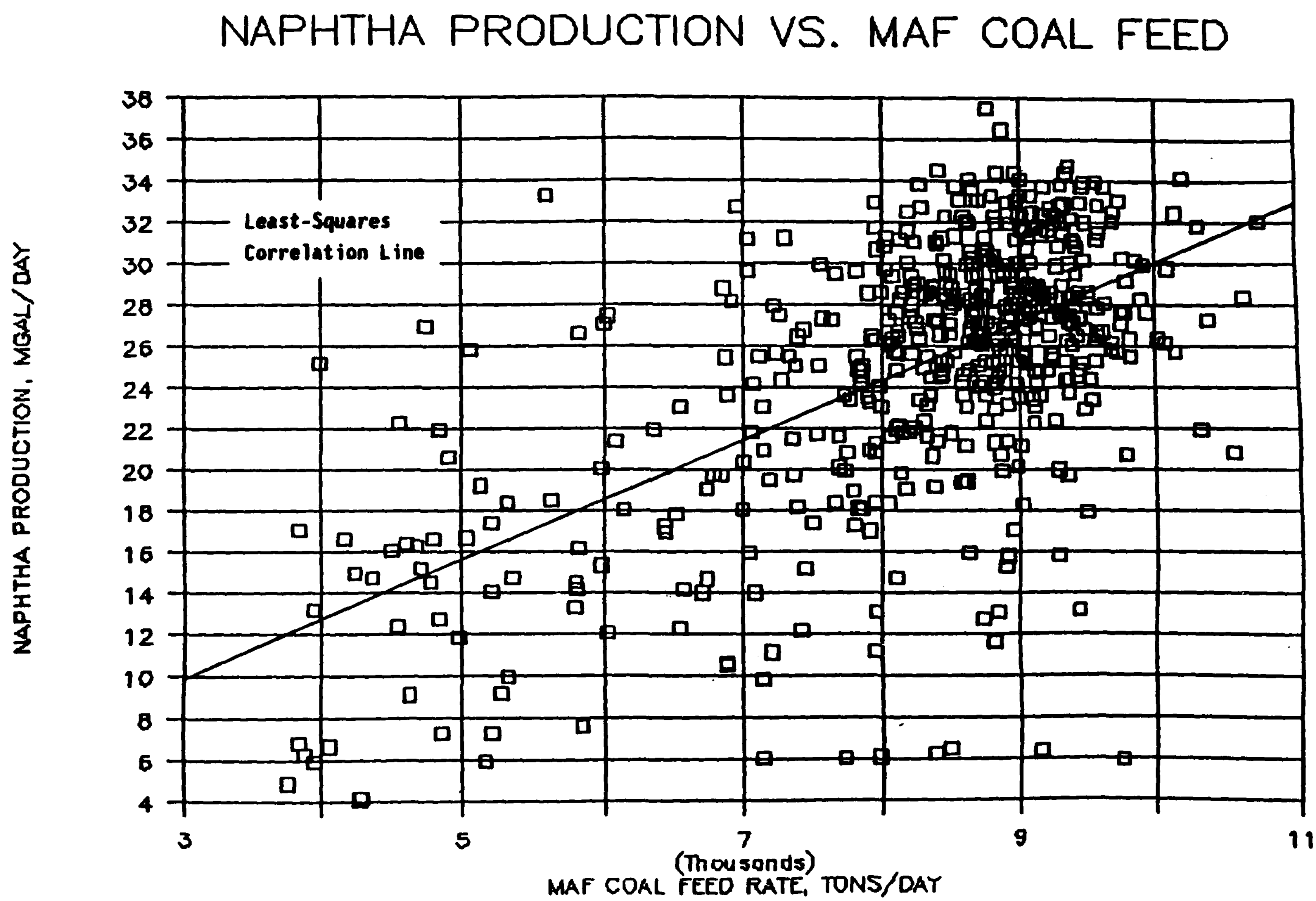

FIGURE A-3. Naphtha Production vs. Maf Coal Feed--1985-1986 Data

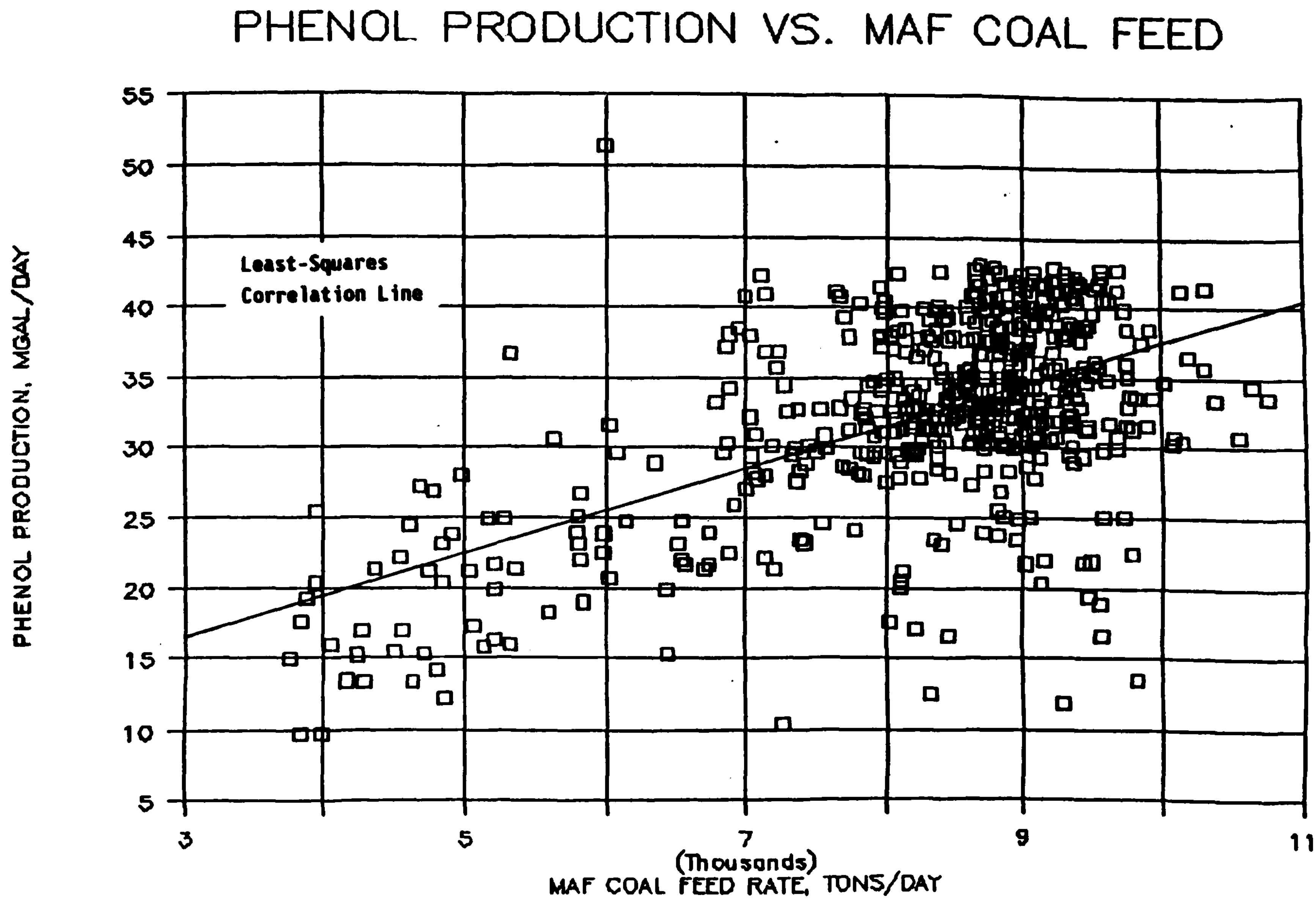

FIGURE A-4. Phenol Production vs. Maf Coal Feed--1985-1986 Data

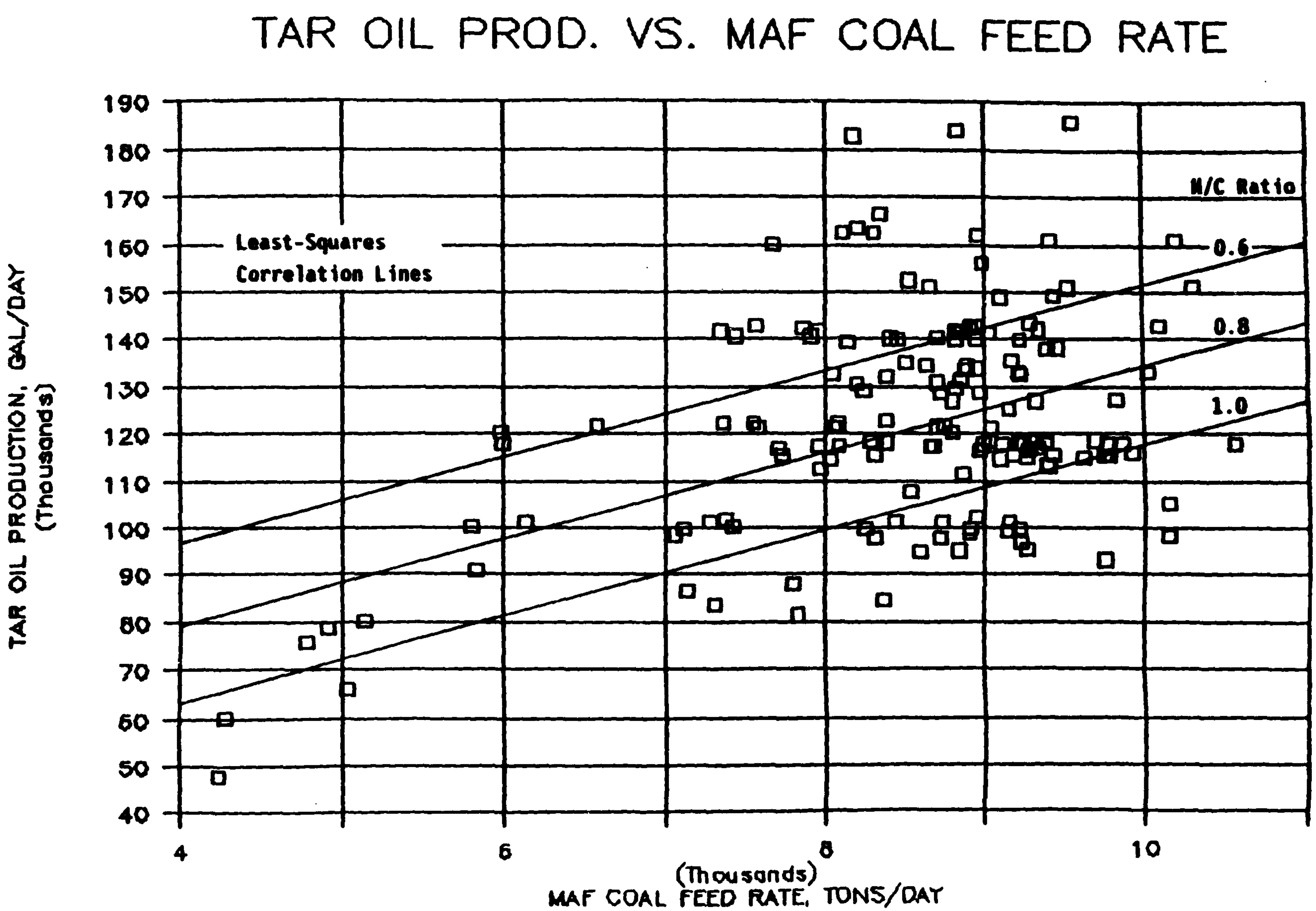

FIGURE A-5. Tar Oil Production vs. Maf Coal Feed Rate and Parameter H/C Ratio--1985-1986 Data

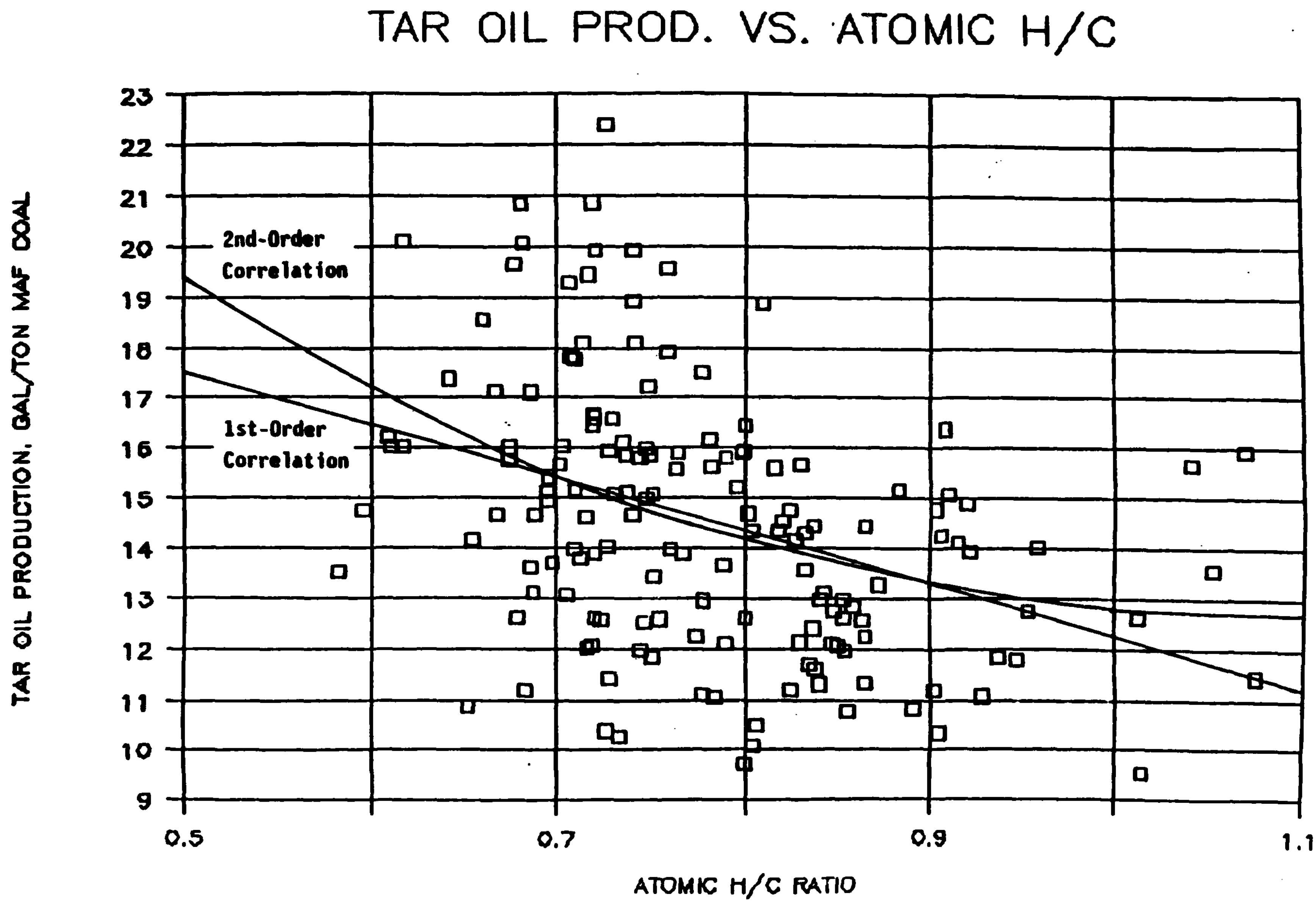

FIGURE A-6. Tar Oil Production vs. Atomic H/C--1985-1986 Data

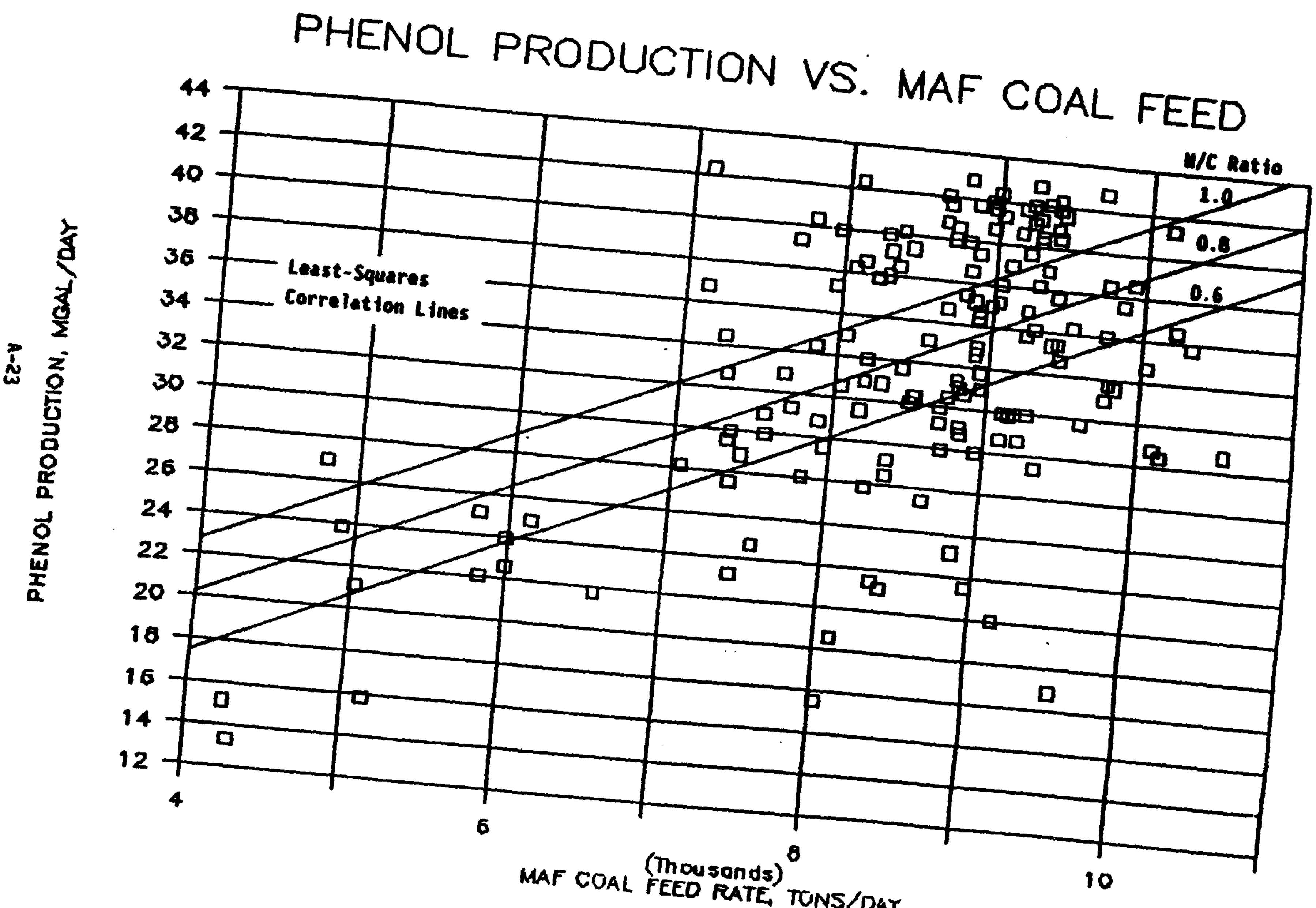

FIGURE A-7. Phenol Production vs. Maf Coal Feed--1985-1986 Data

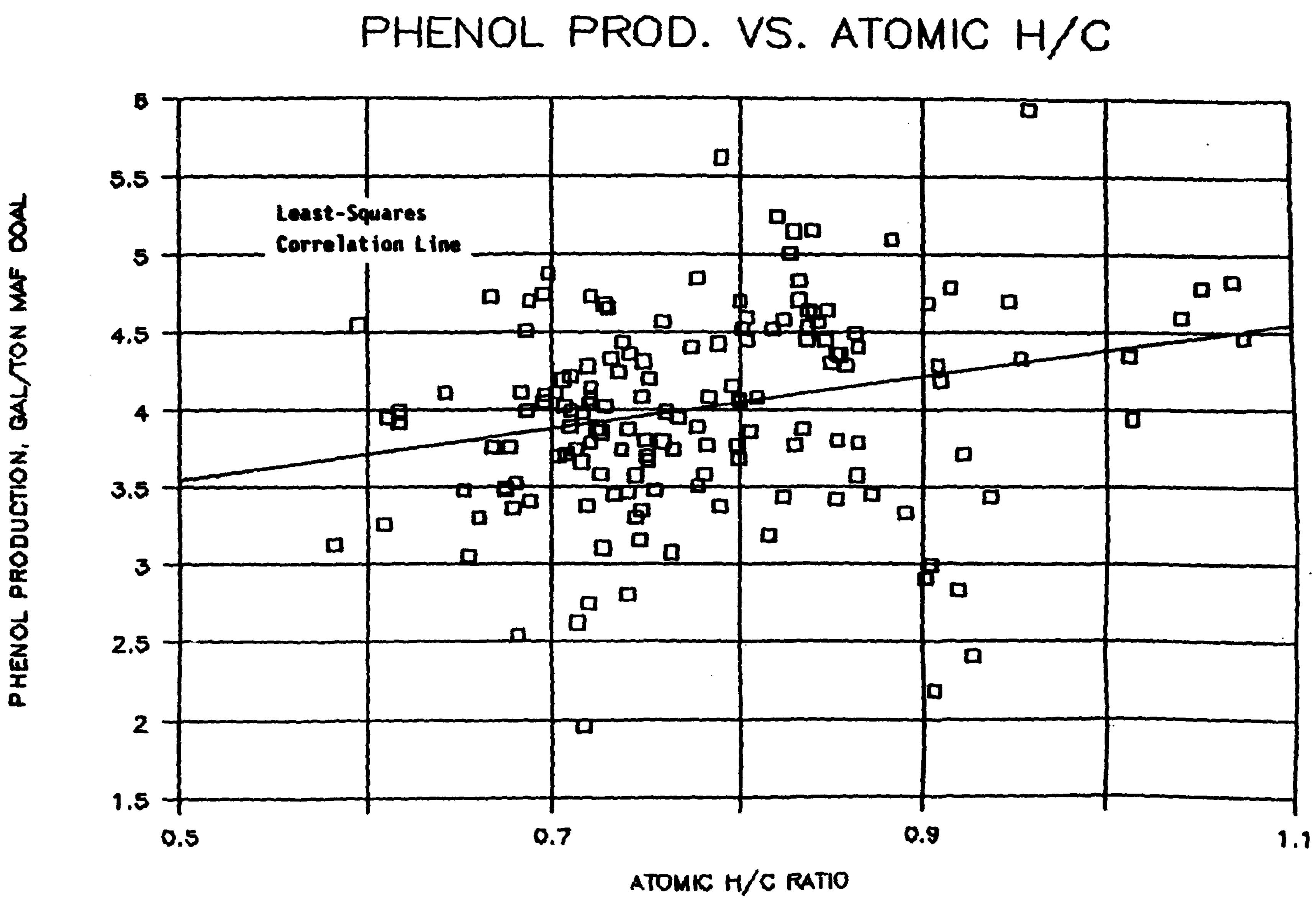

FIGURE A-8. Phenol Production vs. Atomic H/C--1985-1986 Data